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Theoretical Strength of a Perfect Crystal[*]

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A mathematical procedure is presented for applying the Born stability criteria to the determination of the mechanical stability of cubic crystals in the presence of applied forces and deformations. The general procedure presented is suitable for use in conjunction with an electronic computer and is independent of the specific model of interatomic interactions which may be used in numerical calculations. In the present study, specific calculations are performed for a body-centered-cubic (bcc) crystal lattice with an uniaxial force applied perpendicular to a face of a unit cell. The atoms in the crystal are assumed to interact via the two-body Morse interatomic-potential function determined by Girifalco and Weizer [Phys. Rev. 114, 687 (1959)] for bcc iron. Two ranges of stability, a bcc phase and a body-centered-tetragonal (bct) phase, were found to exist. The bct phase has a theoretical strength of 0.9×10^{11} dyn/cm^2 with a corresponding theoretical strain of about 7%. These values are fairly close to the values of 1.3×10^{11} dyn/cm^2 tensile strength and about 5% strain experimentally observed for iron whiskers.

I. INTRODUCTION

Necessary conditions for the thermodynamic stability of a crystal lattice are that the crystal be mechanically stable with respect to arbitrary (small) homogeneous deformations. These conditions are often referred to as the "Born stability criteria" after Born[1] who derived mathematical expressions for these stability requirements for cubic lattices of the Bravais type on the assumption of central forces of a very general type. Misra[2] applied the Born stability criteria to the study of mechanical stability of cubic crystals with inverse-power-law interactions between atoms, and more recently the present author[3] used these criteria to study the stability of cubic crystals with Morse-potential interatomic interactions. These studies were for unstressed (and hence undeformed) crystal lattices.

The present paper is concerned with applying the Born stability criteria to the study of mechanical stability of cubic crystals which are deformed homogeneously under the application of external forces. This study is of interest because the values of stress and strain at which the crystal becomes mechanically unstable, in terms of the Born criteria, represent the "theoretical strength" of the crystal.[4] The failure of a real material under the influence of applied stresses occurs as a result of the strength of the "weakest" region of the lattice being exceeded; this region will evidently be "imperfect." Thus, the limiting value, or upper bound to the strength of a crystalline material, is apparently the strength at which the perfect lattice would fail. Since the perfect lattice, by definition, is homogeneous throughout, it would not fail at some local weak spot, but would, instead, fail as a result of the lattice as a whole becoming mechanically unstable. This instability occurs when the system, consisting of the (deformed) lattice in the presence of the applied forces, can lower its total energy by spontaneously undergoing an additional arbitrary set of small uniform deformations (or strains).

The problem of calculating the theoretical strength of an ideal crystal (i.e., a crystal free of defects) has been studied by several investigators.[5-9] Before the development of the dislocation theory of solids, this problem was of considerable interest because of the fact that calculated values of strength were typically greater than experimental values by a factor of 100 or more. Currently, this problem is still of theoretical as well as practical interest because (a) there now exists the means for obtaining high-strength crystalline whiskers which are evidently relatively free of microscopic defects and (b) the theoretical strength of ideal crystals apparently represents an upper bound to the actual strength of crystalline materials.

Born and Furth[7] applied the Born stability criteria to investigate the theoretical strength of a face-centered-cubic (fcc) crystal lattice for the particular case in which the external force is applied in a direction parallel to a cube edge of a unit cell and in which the atoms in the crystal interact via a two-body inverse power potential; in particular, numerical calculations were performed for a Lennard-Jones 6-12 potential. This investigation was carried out before the advent of electronic digital computers; since the amount of calculation involved is fairly large, at that time it would have been more difficult to perform calculations for other forms of interactions between atoms or other modes of applied lattice deformation.

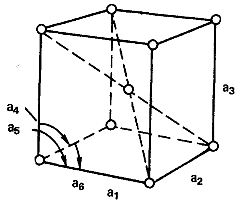
Thus, it is of interest to study the mechanical stability of crystals with various modes of deformation applied and with various forms of interactions between atoms. Present knowledge of interatomic interactions in solids is probably insufficient to allow accurate quantitative calculations of theoretical strength to be made for most crystalline solids. Nevertheless, by using simplified interatomic-interaction models such as an empirical two-body interaction law (as used by Born and Furth) or perhaps a pseudopotential model,[10] it is possible to gain qualitative or semiquantitative information about the theoretical strength of crystals. Similar approaches have been taken by other authors to the study of many phenomena occurring in the solid state. For example, empirical pairwise-interatomic-potential functions (such as the inverse power or Morse functions) have been used to study elastic properties of metals[11,12] and alloys,[13] lattice distortion at surfaces,[14,15] the defect structure of solids including point defects[16,17] and dislocations,[18,19] and the variation of lattice energy in crystals with compression or expansion.[20] Despite the recognition that the interatomic-potential functions are purely empirical and that many-body interactions may play a significant role, such an approach is useful for the following reasons: (i) The interatomic model is inherently fairly simple and thereby allows detailed calculations of many properties of solids to be made; (ii) more rigorous quantum-mechanical solutions are not available for a wide variety of solids; (iii) the potential parameters are chosen to fit some specific experimental data and thereby accurately reflect some definite aspects of the crystal's behavior; and (iv) the use of this model can lead to greater qualitative and often quantitative insight into the nature of the phenomenon being studied.

In the present paper, a mathematical procedure is presented for applying the Born stability criteria to the determination of the mechanical stability of cubic crystals in the presence of applied forces and deformations. The general procedure presented is independent of the specific model of interatomic interactions which may be used in numerical calculations. A specific crystal model and type of applied loading are then selected for stability (i.e., theoretical strength) calculations; the results of these calculations are presented herein. In particular, calculations are performed for a body-centered-cubic (bcc) crystal lattice with a uniaxial force applied perpendicular to a face of a unit cell. The atoms in the crystal are assumed to interact via the two-body Morse interatomic-potential function; the potential parameters used in the present calculations are those determined by Girifalco and Weizer[11] for bcc iron. This particular potential was selected as an initial "test potential" because (a) the potential has a fairly simple mathematical form, (b) the numerical values of the potential parameters were readily available in the literature, and (c) as is concluded by Girifalco and Weizer, "for cubic metals, the Morse potential can be applied to problems involving any kind of a lattice deformation... ."

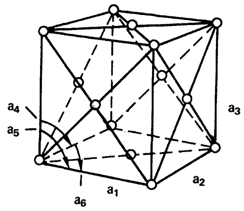
II. THEORY

A. General Theory

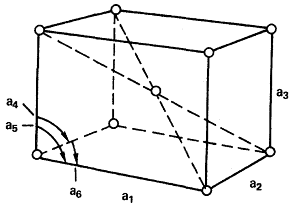
For a simple-crystal lattice which is homogeneously deformed by the application of external forces, the internal energy may be expressed in



(a)
bcc CRYSTAL IN THE ABSENCE OF APPLIED STRESS. Cube Edges $a_1 = a_2 = a_3 = a^\circ$, and angles between edges $a_4 = a_5 = a_6 = \pi/2$.



(b)
fcc CRYSTAL IN ABSENCE OF APPLIED STRESS.
$a_1 = a_2 = a_3 = a^\circ$
$a_4 = a_5 = a_6 = \pi/2$.



(c)
bcc CRYSTAL WITH NORMAL STRESS APPLIED TO THE PLANE PERPENDICULAR TO THE a_1 AXIS.
$a_2 = a_3 \neq a_1$
$a_4 = a_5 = a_6 = \pi/2$.

FIG. 1. Convenient unit cells for bcc and fcc crystals.

terms of the internal energy per unit cell. The energy per unit cell may in turn be expressed as a function of six independent variables that describe the unit cell. Figures 1(a)–1(c), respectively, illustrate convenient unit cells for bcc and fcc crystals, in the state of zero stress, and that of a bcc crystal with a normal stress applied parallel to an edge of the cube. The variables a_i, $i=1, 2, \ldots, 6$ describe the unit cell; a superscript "0" is used to denote the values of the lattice parameters in the absence of applied forces; thus in the state of zero stress, the three cube edges are $a_1^0 = a_2^0 = a_3^0 = a^0$, and the angles between these edges are $a_4^0 = a_5^0 = a_6^0 = \frac{1}{2}\pi$. When the crystal is stressed, the lattice will deform, and each a_i^0 will become a_i, where in the most general case, the edges $a_1 \neq a_2 \neq a_3$ and the angles between the edges $a_4 \neq a_5 \neq a_6 \neq \frac{1}{2}\pi$.

For applied stresses that are large enough to cause failure of the ideal crystal, the deformation[21] of the crystal (and hence of the unit cell) $\{a_i - a_i^0\}$, in general, may not be small compared with a_i^0. Thus, it will be necessary to use a formalism capable of dealing with large deformations. This formalism will be discussed below. The following notation will be used to express the energy per unit cell of the lattice:

$$E(a_1^K, a_2^K, a_3^K, a_4^K, a_5^K, a_6^K) = E)_{\{a_i^K\}} , \tag{1}$$

i.e., $E)_{\{a_i^K\}}$ is the internal potential energy per unit cell evaluated for a specific set of lattice parameters $\{a_i^K\}$, $i=1, 2, \ldots, 6$.

In order for the lattice to be in equilibrium in the state $\{a_i^K\}$, there must be an equilibrium of forces between the externally applied forces and the internal forces resulting from the mutual potential energy of the atoms. This equilibrium is identically satisfied if the "generalized forces" F_i^K acting on the lattice in the state $\{a_i^K\}$ are given by[22]

$$F_i^K = \left(\frac{\partial E}{\partial a_i}\right)_{\{a_i^K\}} , \quad i=1, 2, \ldots, 6 \tag{2}$$

where the F_i^K are defined such that the work involved in a small deformation of the lattice $\{\delta a_i^K\}$ in the state $\{a_i^K\}$ is given by

$$\delta W = \sum_{i=1}^{6} F_i^K \delta a_i^K . \tag{3}$$

These "generalized forces" may be related to the more usual definitions of stress in a fairly straightforward manner. Thus, for example, if an edge a_b^K is elongated by a small amount δa_b^K, holding all other a_i^K constant, the increment of work is given by[23]

$$\delta W = F_b \delta a_b ;$$

clearly this is the work required to move the face (of the unit cell) bordered by the remaining edges a_c and a_d a distance δa_b in the direction of a_b. Thus, F_b must be equal to the force acting on the face (of the unit cell) defined by a_c and a_d in the direction parallel to a_b. Note that δa_b (the deformation measured with respect to the equilibrium value a_b) is small in the above argument; however, the deformation $(a_b - a_b^0)$ or the deformations $\{a_i - a_i^0\}$ (i.e., a_b and the other a_i measured with respect to the equilibrium values of the lattice parameters $\{a_i^0\}$ in the state $F_i^0 = 0$, $i=1, 2, \ldots, 6$) may be arbitrarily large.

For the special case in which the edges of the unit cell a_i, $i=1, 2, 3$ are orthogonal, F_b may be related to the normal stress acting on the plane (of the unit cell) defined by the two edges a_c and a_d (i.e., the plane perpendicular to a_b) by

$$\sigma_b = F_b / a_c a_d ,$$

where b, c, d are permutations of 1, 2, 3. Thus, under the condition of equilibrium of forces, Eq. (2), the normal stress acting on a face of the unit cell when the cell edges are perpendicular to each other is given by

$$\sigma_b^K = \frac{1}{a_c^K a_d^K} \left(\frac{\partial E}{\partial a_b}\right)_{\{a_i^K\}} , \tag{4}$$

where b, d, c are permutations of 1, 2, 3.

For the case in which the cube edges depart only slightly from orthogonality, Eq. (4) still represents, to the first order, the normal stress σ_b^K. In this case, using an argument similar to that leading to Eq. (4), the shear stresses on the faces of the unit cell can be related to the derivatives of E by the relation

$$\sigma_i^K = \frac{1}{(a_1^K a_2^K a_3^K)} \left(\frac{\partial E}{\partial a_i}\right)_{\{a_i^K\}} , \quad i = 4, 5, 6 \tag{5}$$

where, for example, if $i=6$ and a_6 is the angle between a_1 and a_2, σ_6^K represents the shear stress on the plane normal (or approximately normal) to a_2 in the a_1 direction.

Equation (2) thus gives the conditions for the lattice to be in equilibrium with respect to internal and external forces. However, in order for the lattice to be in a stable equilibrium, there is an additional constraint, viz., that the total energy of the system consisting of the lattice in the presence of the applied forces must be at a minimum. In other words, if the state of the lattice specified by the six components $\{a_i^K\}$ is one of stable equilibrium, there must be required a positive expenditure of energy to go from the state $\{a_i^K\}$ to any nearby state $\{a_i^l\}$. This energy expenditure is equal to the difference in the internal potential energy between the state $\{a_i^l\}$ and the state $\{a_i^K\}$ plus the work done by the lattice on its surroundings (i.e., the negative of the work done by the external forces on the lattice). The difference in the internal potential energy between the states $\{a_i^l\}$ and $\{a_i^K\}$ is expressed in terms of a Taylor's series expansion

$$E)_{\{a_i^l\}} - E)_{\{a_i^K\}} = \sum_{i=1}^{6} \left(\frac{\partial E}{\partial a_i}\right)_{\{a_i^K\}} (a_i^l - a_i^K)$$

$$+ \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} \left(\frac{\partial^2 E}{\partial a_i \, \partial a_j}\right)_{\{a_i^K\}} (a_i^l - a_i^K)(a_j^l - a_j^K). \tag{6}$$

The deformations $\{a_i^l - a_i^K\}$ are taken to be small so the series is terminated after second-order terms. (Neither $\{a_i^l - a_i^0\}$ nor $\{a_i^K - a_i^0\}$ is necessarily small, however.) In terms of the definition of equilibrium, the generalized forces acting on the lattice in the state $\{a_i^K\}$ must be $(\partial E/\partial a_i)_{\{a_i^K\}}$; therefore the first term on the right-hand side of Eq. (6) is seen to be identically equal to the work done by the external forces in going from state $\{a_i^K\}$ to state $\{a_i^l\}$. Thus, a positive expenditure of energy will be required for this transition if and only if the second term on the right-hand side of Eq. (6) is positive. For convenience, let

$$\left(\frac{\partial^2 E}{\partial a_i \partial a_j}\right)_{\{a_i^K\}} = B_{ij}^K . \tag{7}$$

According to an algebraic theorem,[24] the double sum in Eq. (6) will be positive for an arbitrary deformation $\{a_i^l - a_i^K\}$ if and only if the principal minors of the determinant $|B_{ij}^K|$ are all positive. Thus, the condition for stable equilibrium is that the determinants of the matrices of successive orders as marked out below (the principal minors) are all positive,

$$[B_{ij}]^K = \begin{bmatrix} B_{11} & B_{12} & B_{13} & B_{14} & B_{15} & B_{16} \\ B_{21} & B_{22} & B_{23} & B_{24} & B_{25} & B_{26} \\ B_{31} & B_{32} & B_{33} & B_{34} & B_{35} & B_{36} \\ B_{41} & B_{42} & B_{43} & B_{44} & B_{45} & B_{46} \\ B_{51} & B_{52} & B_{53} & B_{54} & B_{55} & B_{56} \\ B_{61} & B_{62} & B_{63} & B_{64} & B_{65} & B_{66} \end{bmatrix}^K . \tag{8}$$

(The notation $[B_{ij}^K] = [B_{ij}]^K$ is employed, for convenience.)

If these principal minors are not all positive in the state $\{a_i^K\}$, in which an equilibrium of forces exists, then there exists a state $\{a_i^l\}$ into which the lattice will transform (since it can "liberate" energy by doing so). However, there will not be an equilibrium of forces in the state $\{a_i^l\}$, since the external forces F_i^K have been held equal to $(\partial E/\partial a_i)_{\{a_i^K\}}$, whereas the internal forces have become equal to $(\partial E/\partial a_i)_{\{a_i^l\}}$. The crystal will of course fail under this imbalance of external and internal forces.

In applying the above formalism to a specific crystal, one way to proceed would be to select arbitrarily various sets of $\{a_i\}$, to calculate (for each set $\{a_i\}$) the external forces F_i, Eq. (2), that must be applied in order for the lattice to be in equilibrium in the state $\{a_i\}$, and to calculate the B_{ij} and examine the principal determinants of the matrices B_{ij} (for each set $\{a_i\}$) in order to determine if the lattice is stable in the state $\{a_i\}$.[25] Proceeding in this manner, one could presumably determine a surface in the six-dimensional space of a_i representing the failure criterion of the crystal. This surface would be constructed such that if a specific set of values $\{a_i\}$ were to lie on one side of the surface, the lattice would be stable in this state; as soon as a set of a_i "passed through" this surface, the crystal would fail.

In practice, however, even with the use of electronic computers, the amount of calculation that would be required in order to determine a surface of this sort is fairly large. Thus, one could proceed instead by determining specific points of special interest upon this surface. Such a point may be found by determining a path or a curve to be followed (in the six-dimensional space a_i) that will pass from the stability side of this surface to the side of instability at the point of failure, specified by, say, the set $\{a_i^F\}$. The path to be followed may be defined either by placing constraints directly upon the a_i (e.g., a path could be specified by the constraints $a_1 = a_2 = a_3$ and $a_4 = a_5 = a_6 = \frac{1}{2}\pi$; this would correspond to pure hydrostatic pressure applied to the crystal), or by placing the constraints upon the applied forces F_i. In either case, the set $\{a_i^F\}$ at which the stability criteria becomes violated is found by examining the stability criteria for sets of values $\{a_i\}$ that lie on the particular path (i.e., that are subject to the specified constraints).

It is easier to place the constraints directly upon the a_i since once a set $\{a_i\}$ is specified, the F_i and the B_{ij} may be calculated from Eqs. (2) and (7). However, from a physical point of view, it is usually more interesting to place constraints upon the F_i. (For example, a constraint placed upon the F_i might be the specification that the state $\{a_i\}$ correspond to a state in which a uniaxial force is applied to the crystal; this particular case is considered in greater detail in Sec. II B.) If the forces F_i are constrained to certain values, then it is necessary to determine the set of values $\{a_i\}$ subject to the conditions that $(\partial E/\partial a_i)$, evaluated for the crystal in the state $\{a_i\}$ be equal to the F_i, $i = 1, 2, \ldots, 6$. If for a given set of forces F_i^s a "starting set" $\{a_i^s\}$ is known, additional states $\{a_i\}$ (subject to constraints upon the F_i) may be found by using the iteration procedure presented below. (A convenient "starting set" is the set $\{a_i^0\}$ for which all $F_i^0 = 0$.)

Using the set of values $\{a_i^s\}$, the B_{ij}^s are evaluated [Eq. (7)]. In order to find a nearby state $\{a_i^K\}$ satisfying the conditions of force equilibrium in the presence of a specified set of applied forces F_i^K, Eq. (6) is rewritten as

$$E)_{\{a_i^K\}} = E)_{\{a_i^s\}} + \sum_{i=1}^{6} F_i^s \cdot (a_i^K - a_i^s) + \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} B_{ij}^s \cdot (a_i^K - a_i^s)(a_j^K - a_j^s) \ , \tag{9}$$

and differentiated with respect to a_i^K to obtain

$$F_i^K = \left(\frac{\partial E}{\partial a_i}\right)_{\{a_i^K\}} = F_i^s + \frac{1}{2}\left(\sum_{j=1}^{6} B_{ij}^s \cdot (a_j^K - a_j^s) + \sum_{j=1}^{6} B_{ji}^s \cdot (a_j^K - a_j^s)\right) \ . \tag{10}$$

Taking into account that internal energy is a "state function" independent of path so that $B_{ij} = B_{ji}$, Eq. (10) becomes

$$F_i^K = F_i^s + \sum_{j=1}^{6} B_{ij}^s \cdot (a_j^K - a_j^s), \quad i = 1, 2, \ldots, 6. \tag{11}$$

Thus, given a state $\{a_i^s\}$ in which the equilibrium applied forces F_i^s are known, the general problem of finding a nearby state $\{a_i^K\}$ in which the equilibrium forces are specified as F_i^K, reduces to one of solving the linear system of equations summarized in Eq. (11). After finding the $\{a_i^K\}$, the B_{ij}^K can be evaluated; the "new starting point" can then be taken to be the state $\{a_i^K\}$ [i.e., B_{ij}^K, F_i^K, and a_i^K are substituted for B_{ij}^s, F_i^s, and a_i^s, respectively, in Eqs. (11), and this procedure can be repeated in order to determine a new equilibrium state, say $\{a_i^l\}$, for a new set of external forces, F_i^l].

The above process can be repeated until a set B_{ij}^F is found that violates the stability criteria. The $\{a_i^l - a_i^K\}$ for any successive iteration must, of course, be small with respect to $\{a_i^K\}$; however, the $\{a_i^F - a_i^s\}$ may become relatively large after several iterations.

B. Case of Uniaxial Force

Now, as a specific application of the above formalism, consider a cubic crystal with a uniaxial force applied perpendicular to a cube face, parallel to, say, the edge a_1. In the absence of applied shear stresses, the components a_4, a_5, and a_6 will retain their initial values of $\frac{1}{2}\pi$ (at least up until failure occurs). For a tensile force, the edge a_1 will elongate and the edges a_2 and a_3 will contract; by symmetry it is seen that the relation $a_2 = a_3$ will be maintained. (The deformed crystal will possess tetragonal symmetry.)

An equilibrium state $\{a_i^K\}$ must satisfy the conditions of force equilibrium

$$\left(\frac{\partial E}{\partial a_i}\right)_{\{a_i^K\}} = 0, \quad i \neq 1 \tag{12}$$

and

$$\left(\frac{\partial E}{\partial a_1}\right)_{\{a_i^K\}} = F_1^K \ , \tag{13}$$

where

$$a_2^K = a_3^K \ , \tag{14}$$

$$a_4^K = a_5^K = a_6^K = \tfrac{1}{2}\pi \ , \tag{15}$$

and F_1^K is the applied load. The normal stress in the a_1 direction is simply

$$\sigma_1^K = F_1^K / (a_2^K)^2 \ . \tag{16}$$

As a result of the symmetry of the crystal structure, for $i = 4, 5, 6$ the equations summarized in relation (12) are identically satisfied [since $\partial E/\partial a_4 = \partial E/\partial(-a_4)$, etc.] and for $i = 2$ and 3 these equations are identical to each other. Hence, the relations (12) will be satisfied if

$$\left(\frac{\partial E}{\partial a_2}\right)_{\{a_i^K\}} = 0 \ . \tag{17}$$

Thus, in this case, the problem of finding an equilibrium state $\{a_i^K\}$ reduces to determining a_1^K and a_2^K, subject to Eqs. (13) and (17).

Furthermore, the special symmetry of the crystal in this case also greatly simplifies the matrix $[B_{ij}]$. The following relationships are seen to occur:

$$B_{ij} = B_{ji} \quad , \tag{18}$$

$$B_{ij} = 0 \text{ if } j = 4,\ 5,\ 6 \text{ and } i \neq j \quad , \tag{19}$$

$$B_{22} = B_{33} \text{ and } B_{55} = B_{66} \quad . \tag{20}$$

For example, Eq. (19) can be demonstrated from

$$\frac{\partial^2 E}{\partial a_i\, \partial a_j} = \frac{\partial^2 E}{\partial a_i\, \partial(-a_j)} \, ,$$

$$j = 4,\ 5, \text{ or } 6 \text{ and } i \neq j, \text{ etc.} \tag{21}$$

The matrix $[B_{ij}]$ then takes the form

$$[B_{ij}] = \begin{bmatrix} B_{11} & B_{12} & B_{12} & 0 & 0 & 0 \\ B_{12} & B_{22} & B_{23} & 0 & 0 & 0 \\ B_{12} & B_{23} & B_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & B_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & B_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & B_{55} \end{bmatrix} \tag{22}$$

The principal minors in the determinant of the above matrix will be positive if

$$B_{55} > 0 \quad , \tag{23}$$

$$B_{44} > 0 \quad , \tag{24}$$

$$B_{22} > 0 \quad , \tag{25}$$

$$\begin{vmatrix} B_{22} & B_{23} \\ B_{23} & B_{22} \end{vmatrix} > 0 \quad , \tag{26}$$

$$\begin{vmatrix} B_{11} & B_{12} & B_{12} \\ B_{12} & B_{22} & B_{23} \\ B_{12} & B_{23} & B_{22} \end{vmatrix} > 0 \tag{27}$$

Lattices with Central Pairwise Interatomic Forces

Further simplifications in the above relations result from the approximation of pairwise central forces; in this approximation B_{12}^K and B_{23}^K are equal to $(a_1^K a_2^K)^{-1} B_{55}^K$ and $(a_2^K a_3^K)^{-1} B_{44}^K$, respectively [see Eqs. (56) and (57)], so relations (23) and (24) are equivalent to

$$B_{12} > 0 \tag{28}$$

and

$$B_{23} > 0 \quad . \tag{29}$$

Relations (25), (26), and (29) then imply

$$B_{22} - B_{23} > 0 \quad , \tag{30}$$

and relation (27) leads to

$$B_{11}(B_{22} + B_{23}) - 2(B_{12})^2 > 0 \quad . \tag{31}$$

Relations (28)–(31) *are the necessary and sufficient conditions for the lattice to be in stable equilibrium in terms of the Born criteria.*

In the above case, the remaining symmetry of the crystal in the presence of the applied forces results in a considerable simplification of the iteration procedure for determining the values of the lattice parameters. Equations (11) reduce to

$$F_1^K = F_1^s + B_{11}^s \cdot (a_1^K - a_1^s) + 2B_{12}^s \cdot (a_2^K - a_2^s) \tag{32}$$

and

$$\begin{aligned} F_2^K &= 0 \\ &= B_{12}^s \cdot (a_1^K - a_1^s) + (B_{22}^s + B_{23}^s) \cdot (a_2^K - a_2^s) \quad ; \end{aligned} \tag{33}$$

upon rearranging Eq. (33),

$$a_2^K - a_2^s = -[B_{12}^s / (B_{22}^s + B_{23}^s)]\ (a_1^K - a_1^s) \quad , \tag{34}$$

and substituting Eq. (34) into Eq. (32),

$$F_1^K = F_1^s + [B_{11}^s - 2(B_{12}^s)^2 / (B_{22}^s + B_{23}^s)]\ (a_1^K - a_1^s). \tag{35}$$

The iteration process may begin with the known values of the lattice parameters $a_1^s = a_2^s = a^0$ for which all $F_i^s = 0$. After calculating the values of B_{ij}^s, the lattice parameter a_1 is elongated by a small amount $a_1^K - a_1^s$. The value of a_2^K (for which $F_2^K = 0$) is then found from Eq. (34); the value F_1^K (which "results in the elongation" $a_1^K - a_1^s$) may be determined from Eq. (35), or may be calculated directly from Eq. (2). The B_{ij}^K are evaluated for these values of lattice parameters and the process is repeated for another incremental elongation $a_1^l - a_1^K$ of a_1. This is continued until one of the stability relations is violated. The value of $F_1^F/(a_2^F)^2$ at which the instability occurs is the theoretical strength (stress) of the crystal and $(a_1^F - a_1^0)/a_1^0$ is the theoretical maximal strain.

C. Numerical Calculations in Model of Central Pairwise Interatomic Interactions

In the previous discussion, the means of determining an equilibrium state of the lattice $\{a_i\}$ in the presence of generalized forces F_i is outlined in detail. It has been assumed implicitly that for a given set of lattice parameters $\{a_i\}$ the quantities F_i [Eq. (2)] and B_{ij} [Eq. (7)] can be calculated. In this section the calculation of these quantities for a particular model of a cubic crystal, viz., one in which the atoms interact in a central pairwise manner, is discussed. As was mentioned earlier, this model has been used by many authors[11–20] in investigations of a wide variety of solid-state phenomena. A basic assumption is that the potential energy of interaction between two atoms $\phi(r_{ij})$ may be written as a function of the interatomic spacing r_{ij} between the atoms. The conditions which "any potential function $[\phi]$ must satisfy if it is to describe reality" have been discussed in detail by Girifalco and Weizer.[11] In Sec. III, explicit numerical results are presented for calculations carried out for a bcc crystal lattice using the well-known Morse function,

$$\phi(r_{ij}) = D\,[e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}] \ . \tag{36}$$

The potential parameters used in the calculations are those which have been determined for bcc iron[11]; this potential satisfies each of the requisite conditions discussed by Girifalco and Weizer.

In the pairwise interaction model, the energy per unit cell of the lattice may be written as

$$E)_{\{a_i\}} = \tfrac{1}{2} n \textstyle\sum_j \phi[(r_j)_{\{a_i\}}] , \tag{37}$$

where n is the number of atoms per unit cell and r_j is the distance from an arbitrary atom in the lattice (chosen as the origin) to the jth atom; the sum is to be evaluated for a specific set of lattice parameters $\{a_i\}$ and the index j runs over all atoms in the crystal. Of course, in actual calculations, the index j need include only enough terms to obtain convergence to within the desired number of significant figures.

In a bcc or an fcc crystal lattice which is subject to uniform deformations, the vector $\vec{r}_j$ passing from the origin to the jth atom in the crystal may be written as

$$\vec{r}_j = \vec{r}_{l_1 l_2 l_3} = \frac{1}{2} \sum_{i=1}^{3} l_i a_i \hat{a}_i \tag{38}$$

and the square of its magnitude is given by

$$(r_{l_1 l_2 l_3})^2 = \frac{1}{4} \sum_{i=1}^{3} \sum_{j=1}^{3} l_i l_j a_i a_j \hat{a}_i \cdot \hat{a}_j ; \tag{39}$$

the $\hat{a}_i$ are unit vectors in the directions of the cell edges a_i, and the l_i are integers. For a bcc crystal, the l_i run over all integer values for which l_1, l_2, l_3 are either all odd or all even, and for an fcc lattice, the l_i are subject to the conditions that the sum $l_1 + l_2 + l_3$ is even. In this notation, Eq. (37) becomes

$$E)_{\{a_i\}} = \tfrac{1}{2} n \sum_{l_1} \sum_{l_2} \sum_{l_3} \phi\,[(r_{l_1 l_2 l_3})_{\{a_i\}}] , \tag{40}$$

where the sums are performed over all allowed integer values l_i (i.e., until convergence is obtained).

The F_i, Eq. (2), and the B_{ij}, Eq. (7), may then be found by differentiating Eq. (40),

$$\frac{\partial E}{\partial a_i} = \frac{1}{2} n \sum_{l_1} \sum_{l_2} \sum_{l_3} \frac{\partial \phi(r)}{\partial r^2} \frac{\partial r^2}{\partial a_i} , \tag{41}$$

and

$$\frac{\partial^2 E}{\partial a_i \partial a_j} = \frac{1}{2} n \sum_{l_1} \sum_{l_2} \sum_{l_3} \left[\frac{\partial^2 \phi(r)}{(\partial r^2)^2} \cdot \frac{\partial r^2}{\partial a_i} \frac{\partial r^2}{\partial a_j} + \frac{\partial \phi(r)}{\partial r^2} \frac{\partial^2 r^2}{\partial a_i \partial a_j} \right] , \tag{42}$$

where r is taken to mean $(r_{l_1 l_2 l_3})_{\{a_i\}}$, the derivatives are all evaluated for the particular set $\{a_i\}$, and the $\partial\phi/\partial r^2$ and $\partial^2\phi/(\partial r^2)^2$ are found directly from the particular form of two-body potential function that is used. The $\partial r^2/\partial a_j$ and $\partial^2 r^2/\partial a_i \partial a_j$ are evaluated by differentiating Eq. (39), which, when expanded, takes the form

$$r^2 = \tfrac{1}{4} [l_1^2 a_1^2 + 2 l_1 l_2 a_1 a_2 \cos a_6 + 2 l_1 l_3 a_1 a_3 \cos a_5 + l_2^2 a_2^2 + 2 l_2 l_3 a_2 a_3 \cos a_4 + l_3^2 a_3^2] . \tag{43}$$

Thus, for example, some of the derivatives of interest in Eqs. (41) and (42) are

$$\frac{\partial r^2}{\partial a_1} = \tfrac{1}{2} [l_1^2 a_1 + l_1 l_2 a_2 \cos a_6 + l_1 l_3 a_3 \cos a_5] , \tag{44}$$

$$\frac{\partial r^2}{\partial a_4} = -\tfrac{1}{2} l_2 l_3 a_2 a_3 \sin a_4 , \tag{45}$$

$$\frac{\partial^2 r^2}{\partial a_1^2} = \tfrac{1}{2} l_1^2 , \tag{46}$$

$$\frac{\partial^2 r^2}{\partial a_4^2} = -\tfrac{1}{2} l_2 l_3 a_2 a_3 \cos a_4 , \tag{47}$$

$$\frac{\partial^2 r^2}{\partial a_1 \partial a_2} = \tfrac{1}{2} l_1 l_2 \cos a_6 , \tag{48}$$

$$\frac{\partial^2 r^2}{\partial a_1 \partial a_5} = -\tfrac{1}{2} l_1 l_3 a_3 \sin a_5 , \tag{49}$$

$$\frac{\partial^2 r^2}{\partial a_1 \partial a_4} = 0 , \tag{50}$$

$$\frac{\partial^2 r^2}{\partial a_4 \partial a_5} = 0 . \tag{51}$$

For the particular case of a uniaxial tensile stress applied parallel to the a_1 axis ($a_2 = a_3$ and $a_4 = a_5 = a_6 = \tfrac{1}{2}\pi$), the cosines in the above equations are zero and the sines are unity. Equations (41) and (42) then lead to the following lattice sums for the F_i and the B_{ij}:

$$F_i = \tfrac{1}{4} n a_i \sum_{l_1 l_2 l_3} l_1^2 \frac{\partial\phi}{\partial r^2}, \quad i = 1, 2, 3 \tag{52}$$

$$B_{11} = \tfrac{1}{8} n a_1^2 \sum_{l_1 l_2 l_3} l_1^4 \frac{\partial^2\phi}{(\partial r^2)^2} + \tfrac{1}{4} n \sum_{l_1 l_2 l_3} l_1^2 \frac{\partial\phi}{\partial r^2}, \tag{53}$$

$$B_{12} = \tfrac{1}{8} n a_1 a_2 \sum_{l_1 l_2 l_3} l_1^2 l_2^2 \frac{\partial^2\phi}{(\partial r^2)^2}, \tag{54}$$

$$B_{44} = \tfrac{1}{8} n (a_2 a_3)^2 \sum_{l_1 l_2 l_3} l_2^2 l_3^2 \frac{\partial^2\phi}{(\partial r^2)^2}. \tag{55}$$

The remaining B_{ij} may be found by switching subscripts in the above equations. For example, to find B_{22}, a_1 and l_1 are changed to a_2 and l_2 in Eq. (53); for B_{23}, a_1 and l_1 are changed to a_3 and l_3 in Eq. (54); and for $B_{55} = B_{66}$, a_3 and l_3 are changed to a_1 and l_1 in Eq. (55). As a result of the assumption of pairwase central forces, the relations

$$B_{44} = a_2 a_3 B_{23} \tag{56}$$

and

$$B_{55} = a_1 a_2 B_{12} \tag{57}$$

occur, as may be verified by comparison of the respective lattice sums. Any lattice sum that contains an l_i to an odd power will be zero; so terms such as

$$F_6 = -n a_1 a_2 \sum_{l_1 l_2 l_3} l_2 l_3 \frac{\partial\phi}{\partial r^2} = 0 .$$

III. NUMERICAL RESULTS AND DISCUSSION

Section II presented in detail a mathematical procedure for applying the Born stability criteria to the calculation of the mechanical stability of an ideal crystal in the presence of externally applied forces. To obtain numerical results, it is of course necessary to use a particular model for interatomic interactions. In the present study, explicit numerical results are obtained for the particular case of a bcc crystal lattice with two-body Morse-function [Eq. (36)] interactions between atoms. Morse-function interactions have been used by many authors to calculate behavior or properties of solids; e.g., Morse functions have been used to calculate equations of state,[11] elastic moduli of metals[11,12] and alloys,[13] lattice distortion at surfaces,[14,15] the propagation of shock waves in crystals,[26] and characteristics of point defects[27] and dislocations.[19]

The values of the potential parameters used in the present calculations are those determined by Girifalco and Weizer[11] for bcc iron, viz.,

$$D = 0.4174 \text{ eV},$$

$$r_0 = 2.845 \text{ Å},$$

$$\alpha = 1.3885 \text{ Å}^{-1},$$

where the equilibrium value of the lattice parameter $a^0 = 2.8631$ Å. These parameters were determined by fitting the Morse function to experimental values of cohesive energy, compressibility, and the equilibrium lattice parameter of bcc iron. That is, the Morse function, with these particular parameter values, satisfies the following conditions for bcc iron: (i) Substituting the Morse function $\phi(r)$ into Eq. (40) yields a value of $E)_{\{a_i^0\}}$ equal to the experimental value of cohesive energy (at 0 °K); (ii) substituting $\phi(r)$ into the appropriate expression[28] for compressibility yields the respective experimental value; and (iii) substituting $\phi(r)$ into the expression for applied forces, Eq. (52), yields $F_i = 0$ when $\{a_i\} = \{a_i^0\}$.

In the present study, numerical calculations of lattice stability are made for the case of a uniaxial force applied parallel to an edge of the unit cell, parallel to, say, the lattice parameter a_1. In this case, the conditions for lattice stability are given by relations (28)–(31). The quantities in these relations are calculated using the lattice summations of Eqs. (53)–(55). The values of the lattice parameters which are used in evaluating these summations are those for which Eqs. (52) are satisfied, i.e., those which the lattice summations of Eqs. (52) yield F_1 equal to the applied force (per unit cell) and $F_2 = F_3 = 0$. The applied stress $\sigma_1 = F_1/(a_2)^2$. The first and second derivatives of $\phi(r)$ which appear in these lattice summations are

$$\frac{\partial\phi}{\partial r^2} = \frac{-D\alpha}{r}\left[e^{-2\alpha(r-r_0)} - e^{-\alpha(r-r_0)}\right] \tag{58}$$

and

$$\frac{\partial^2\phi}{(\partial r^2)^2} = \frac{D\alpha}{r^2}\left[\left(\alpha + \frac{1}{2r}\right)e^{-2\alpha(r-r_0)} - \left(\frac{1\alpha}{2} + \frac{1}{2r}\right)e^{-\alpha(r-r_0)}\right]. \tag{59}$$

The magnitude of r appearing in these expressions is given by the square root of Eq. (43). The summations are evaluated with the aid of an electronic digital computer; approximately 2000 lattice sites are included in each sum.

Results of numerical calculations of the applied stress σ_1, the internal energy $E)_{\{a_i\}}$ (or simply E), and the stability criteria for the bcc lattice[29] are shown as a function of lattice parameter a_1 in Figs. 2–4. In Fig. 2 it is seen that the applied stress increases from zero at the unstressed equilibrium value of lattice parameter $a_1^0 = 2.8631$ Å to a maximum of 1.7×10^9 dyn/cm^2 at $a_1 = 2.9128$ Å, where the stability criteria are violated. Figure 3

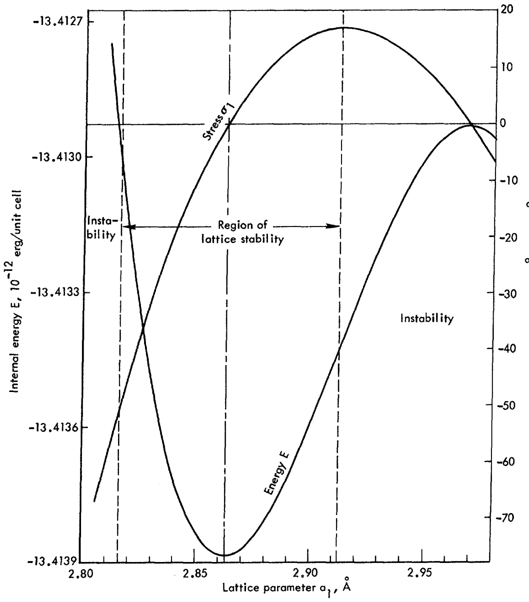


FIG. 2. Internal energy and applied stress as a function of lattice parameter a_1 in the region of stability of the bcc crystal.

shows that it is the stability relation

$$B_{11}[B_{22}+B_{23}] - 2B_{12}^2 > 0$$

which is violated at this point; evidently this relation becomes violated when a further increase in lattice parameter a_1 leads to a decrease in the equilibrium stress σ_1 (or in other words when the lattice cannot accommodate a further increase in applied stress). Thus, in this model, the bcc lattice becomes unstable at a theoretical tensile stress of 1.7×10^9 dyn/cm^2 and a corresponding maximal strain of

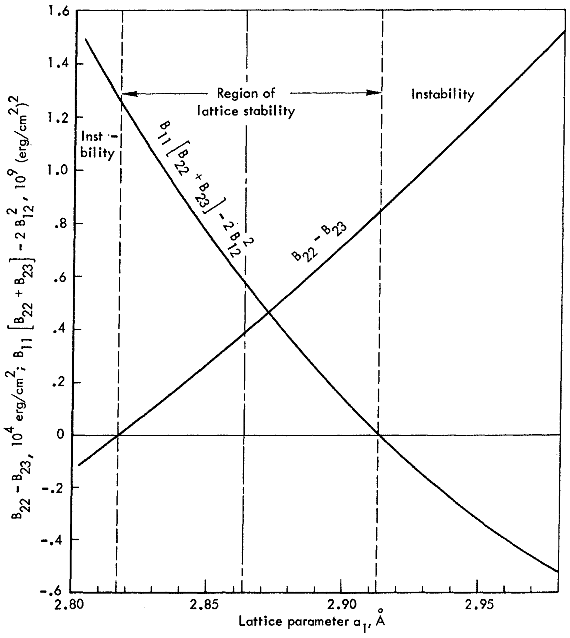


FIG. 3. $B_{11}[B_{22}+B_{23}]-2B_{12}^2$ and $B_{22}-B_{23}$ as a function of lattice parameter a_1 in the region of stability of the bcc crystal. The long-short dashed line indicates the position of stability for zero applied stress.

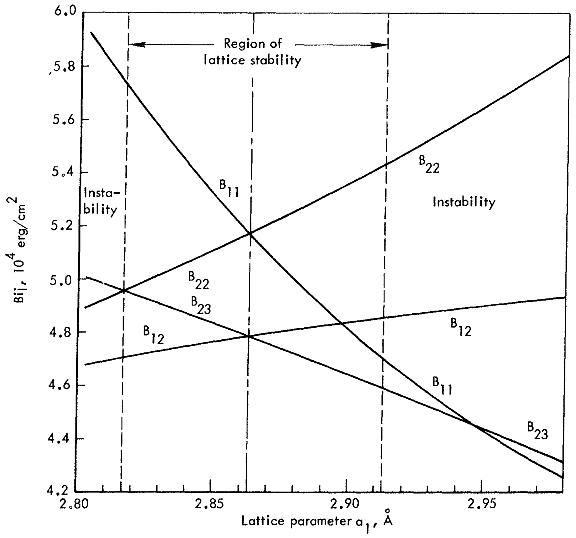


FIG. 4. Independent moduli B_{ij} as a function of lattice parameter a_1 in the region of stability of the bcc crystal. The long-short dashed line indicates the position of stability for zero applied stress.

$$\epsilon_1 = (2.9128 - a^0)/a^0 = 0.01735.$$

In compression, the bcc lattice becomes unstable at an applied stress $\sigma_1 = -5.05 \times 10^9$ dyn/cm^2 at lattice parameter $a_1 = 2.8166$ Å corresponding to a strain $\epsilon_1 = 0.0162$. Figure 3 shows that instability in compression results from the violation of the condition $B_{22} - B_{23} > 0$. The violation of this condition corresponds to the mode of failure by which the crystal can lower its total energy by undergoing spontaneously the following lattice deformation: The lattice parameters a_2 and a_3 deform oppositely by equal amounts (e.g., if a_2, say, increases, then a_3 decreases by the same amount) while a_1 and the angles a_4, a_5, and a_6 remain fixed.

Figure 4 shows the variation of the four independent moduli B_{11}, B_{12}, B_{22}, and B_{23} in the range in which the stressed bcc lattice is stable as a function of lattice parameter a_1. The relations $B_{11} = B_{22}$ and $B_{12} = B_{23}$ occur for $a_1 = a^0$ (i.e., for zero applied stress $a_1 = a_2 = a_3 = a^0$); these relations of course result from the cubic symmetry of the unstressed crystal. None of the individual B_{ij}'s become negative at the points of failure of the stressed bcc lattice [it is noted that the satisfaction of the stability relations (28) – (31) also implies $B_{11} > 0$ and $B_{22} > 0$].

There are several noteworthy aspects to the behavior of the bcc crystal under the influence of the tensile stress σ_1. First, it is noted that the crystal fails at a relatively low value of stress $\sigma_1 = 1.7 \times 10^9$ dyn/cm^2; then, instead of approaching zero asymptotically, the equilibrium (but unstable) value of stress becomes negative. The internal energy E, of course, passes through a maximum at the value of a_1 at which σ_1 becomes negative ($a_1 = 2.9687$ Å). Since the nature of the interatomic-potential function $\phi(r)$ requires that E must ultimately increase (to zero) as a_1 increases, the energy E must pass through another minimum and σ_1 must pass from a negative to a positive value again at some larger value of a_1, say $a_1 = b_1^0$.

Thus at $a_1 = b_1^0$, there exists another crystalline phase, a body-centered-tetragonal (bct) phase, which is in equilibrium in the absence of applied forces; the lattice parameters of this phase (in the unstressed state) are denoted as $a_1 = b_1^0, a_2 = a_3 = b_2^0$, and $a_4 = a_5 = a_6 = \frac{1}{2}\pi$. Some questions of interest regarding the bct phase are: (a) Is this phase (in the unstressed state) at a higher or lower internal energy then the unstressed bcc phase? (b) Does the bct phase exist in a *stable* equilibrium? (c) If it does exist in a stable equilibrium, what are the values of its theoretical strength and maximal strain and what are its modes of failure in tension and in compression? The answers to these questions may be found in Figs. 5 and 6.

Figure 5 shows the lattice parameter a_2 (as determined by the condition $\sigma_2 = 0$), the applied stress σ_1, and the internal energy E over a fairly large range of lattice parameter a_1. The unstressed ($\sigma_1 = 0$) bct phase possesses the lattice parameters $a_1 = b_1^0 = 3.6055$ Å and $a_2 = b_2^0 = 2.5495$ Å corresponding to the minimum of internal energy $E = -13.501 \times 10^{-12}$ erg/unit cell. In Fig. 5 it is seen that the internal-energy minimum of the bct phase is considerably lower than that of the bcc phase (about -13.4139×10^{-12} erg/unit cell). Furthermore, the potential well corresponding to the bcc phase is relatively shallow (hence the relatively small value for the maximum stress of this phase).

Figure 6 shows that at $a_1 = b_1^0$, all of the stability conditions are fulfilled; thus, the bct phase is in *stable* equilibrium in terms of the Born criteria. In this figure it is seen that the bct phase is stable within the range of lattice parameter $a_1 = 3.3375$ Å to $a_1 = 3.8606$ Å. It is noted that the range of stability of the bct phase is considerably greater than that of the bcc phase. From Fig. 5, the theoretical strength of the bct phase is 8.90×10^{10} dyn/cm^2 in tension and -3.22×10^{10} dyn/cm^2 in compression; the corresponding strain $\epsilon_1 = 0.0707$ in tension and -0.0740 in compression. The lattice fails in tension by violating the condition $B_{23} > 0$ and in compression by violating the condition

$$B_{11}[B_{22} + B_{23}] - 2B_{12}^2 > 0 \ .$$

The violation of the latter condition results when the lattice cannot support an additional compressive load (i.e., when a decrease in lattice parameter a_1 results in an increase rather than a decrease in stress σ_1). When the condition $B_{23} > 0$ is violated, the lattice can lower its energy by undergoing a spontaneous deformation wherein the angle a_4 (the angle between a_2 and a_3) deviates from 90°.

It is noted that the bct lattice fails in tension considerably before the maximum equilibrium stress of 4.44×10^{11} dyn/cm^2 is reached; this behavior demonstrates the necessity for examining the stability relations (28)–(31) in order to determine the theoretical strength of the crystal, rather than simply calculating the maximum value of stress and corresponding maximal strain.

Calculations such as those shown in Figs. 5 and 6 were carried out throughout the range of lattice parameter $a_1 = 2.00$ Å to $a_1 = 9.20$ Å; the lattice was found to satisfy the Born criteria only in the bcc and bct regions indicated in Figs. 5 and 6.

It is of interest to comment upon the result that, for the interatomic potential used in the present study (i.e., the Morse function determined by

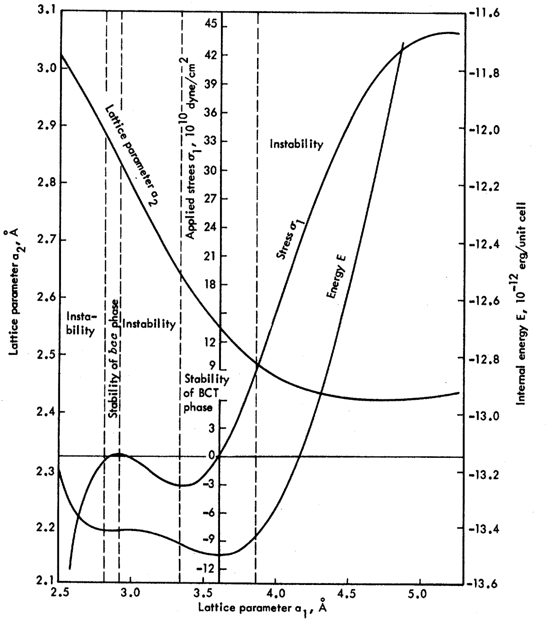


FIG. 5. Internal energy, applied stress, and lattice parameter a_2 as a function of lattice parameter a_1. Regions of lattice stability and instability are separated by short dashed lines. Ordinate and abscissa scales are considerably different from those of Fig. 2.

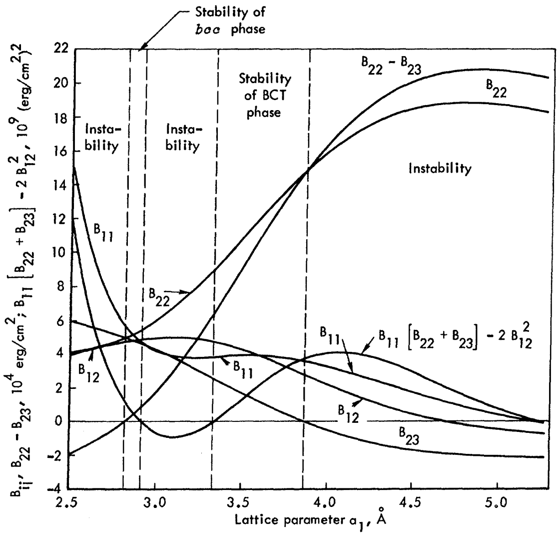


FIG. 6. $B_{11}[B_{22}+B_{23}]-2B_{12}^2$, $B_{22}-B_{23}$, and the four independent B_{ij}'s as a function of lattice parameter a_1. The lattice is unstable in the regions where the numerical values of any of these curves are less than or equal to zero.

Girifalco and Weizer for bcc iron), the bct phase is at a lower energy and is evidently more stable than the bcc phase. Although this result is not in correspondence with the actual behavior of pure iron which exists in the bcc phase, it is interesting to note that when carbon or nitrogen is dissolved into iron, the lattice distorts into the bct form. The lattice parameter a_1 elongates and a_2 and a_3 contract; the carbon or nitrogen atoms occupy interstitial positions midway along the equivalent edges a_1 of the unit cell. As is pointed out by Cottrell,[30] "a study of the bcc cell shows rather surprisingly that these are not the positions of the largest interstitial holes in the cell." Thus iron containing dissolved carbon or nitrogen exists in the bct structure even though, based upon considerations of size alone, this structure is not the one which accommodates the carbon or nitrogen atoms most readily.

In the present calculations the lattice (in the bct phase) was found to remain stable up to a tensile strain of about 7% with a corresponding strength of about 9×10^{10} dyn/cm^2. It is of interest to compare this estimate of theoretical strength and strain with the results of some experimental measurements in which the stress and strain apparently approach the theoretical limit. Crump and Mitchell[31] have recently reported observing elastic strains as high as 4.5% in "nearly perfect" crystals of cadmium. Brenner[32,33] has measured the tensile strength of fine iron whiskers and has reported ultimate tensile strengths of about 13×10^{10} dyn/cm^2 with corresponding strains close to 5%. The values of stress and strain obtained in the present calculations for the bct phase are reasonably close to these experimentally observed values. The theoretical values of stress and strain for the bcc phase, however, are considerably less than the experimental values quoted above.

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[*] Most of this work was done while the author was with the RAND Corp. and later with the School of Engineering and Applied Science, University of California, Los Angeles, Calif.

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[21] The notation { } is used to denote a set of six components; thus $\{a_i - a_i^0\}$ represents a set of six deformations $a_1 - a_1^0$, $a_2 - a_2^0$, ..., $a_6 - a_6^0$. A superscript is used to denote a particular set of values of the lattice parameters, e.g., $\{a_i^K\}$ represents a state of the lattice in which lattice parameter a_1 has the value a_1^K, etc.

[22] The notation $(\partial E/\partial a_i)\{a_i^K\}$ indicates that the partial derivative is to be evaluated for the case in which the lattice parameters have the values $\{a_i^K\}$.

[23] If it is clear that the forces F_i^K and lattice parameters

a_i^K refer to a particular state $\{a_i^K\}$, the superscript K will often be omitted.

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[25] In order to calculate numerically the quantities F_i and B_{ij}, a specific model for interatomic interactions is of course required. The means of evaluating these quantities for the case of central two-body interactions between atoms will be discussed in Sec. II C.

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Debye-Waller Factors of Cubic Metals

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The exponents of the Debye-Waller factor for the cubic metals copper, silver, gold, aluminium, nickel, sodium, chromium, and α-iron are determined at different temperatures from the vibrational spectrum derived from a model for the lattice dynamics of metals recently propounded by Chéveau, which includes the influence of conduction electrons on lattice vibrations. The calculation uses Blackman's root-sampling technique for a discrete subdivision in wave-vector space. The results of the calculations are compared with available experimental data in terms of the Debye-Waller–factor temperature parameter Y, the effective x-ray characteristic temperature Θ_M, and the mean-square displacement of the atoms $\overline{u^2}$. Except for chromium, the theoretical values show reasonably satisfactory agreement with the experimental measurements.

I. INTRODUCTION

In the nonresonant elastic scattering of waves (slow neutrons, x rays, etc.) from scatterers which are bound in crystals, the fall in the intensity on account of lattice thermal motion is governed by an exponential factor e^{-2M}, called the Debye-Waller factor. The exponent $2M$ depends upon the mean-square displacement of the atoms, and can be correlated with many other solid-state phenomena. In the recent past, considerable interest has been shown in the experimental study of the thermal variation of the Debye-Waller factors of metals by means of x-ray diffraction. The experimental data have usually been interpreted in terms of the Debye theory, using volume-change corrections due to Paskin.[1]

It is now well known that electrons in metals influence considerably the vibrational frequencies and their lattice-dynamical behavior. In recent years, a number of models[2-4] have been propounded for calculating the phonon frequencies of metals by taking cognizance of electrons in various approximate ways. However, many of these models violate some symmetry properties of a cubic lattice. Lax[5] has attributed this inadequacy to the neglect of translational invariance of the lattice. Recently, Krebs[6] has attempted to remove this difficulty by considering umklapp processes. However, this model suffers from a serious defect of internal equilibrium, i.e., the derivative of the long-range screened Coulomb interaction energy does not vanish at the equilibrium configuration as it does for the short-range Born–von Kármán term. This necessitates external forces to maintain the system in equilibrium. Quite recently, Chéveau[7] has propounded a model for the dispersion of lattice waves in cubic metals which satisfies the symmetry requirements of a cubic lattice and preserves internal equilibrium without recourse to any external force. The model considers the ion-ion interaction as the first two terms in Taylor expansion of the potential energy. For the electron-ion interaction, the linearized Thomas-Fermi equation is used over the whole crystal. The model has recently been used by the authors[8] to study the thermal variations of the Grüneisen parameters of cubic metals and was found to give