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Principles of stability analysis of ideal crystals

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It is current practice to determine the "strength" profile of an ideal crystal by calculating the domain of homogeneous deformation in which the crystal is classically stable. This approach is here implemented in a less restricted manner than previously: first, by admitting any generalized coordinates to specify the strain; second, by assessing the stability in an arbitrary load environment. From this standpoint the intrinsic subjectivity of the usual concept of strength appears clearly. In illustration divergent estimates of uniaxial strength in the literature are compared within a common framework. With a view to rationalizing the whole approach, the present analysis gives prominence to the objective notion of coordinate invariance. Special "failure" modes, associated with path branchings at a domain perimeter, are also examined in this light. Finally, the stability of purely volumetric deformation is examined in detail.

I. INTRODUCTION

In this paper we aim to clarify the concept of ideal crystal strength, when regarded as an instability phenomenon in the context of classical mechanics. This is the approach initiated in 1940 by Born[1] and extensively developed more recently with the aid of electronic computers (e.g., Basinski *et al.*,[2] Macmillan and Kelly,[3] Milstein,[4,5] Huang *et al.*[6]).

According to Born, any crystal capable of homogeneous deformation may be treated as a conservative dynamical system with six degrees of freedom; stability, in the ordinary Lagrangian sense, is then to be assessed along conventional lines. However, it is in the detail of this theory that different writers have in practice diverged by virtue of choosing different sets of generalized coordinates. This is important because, in a crystal under load, convexity of the internal-energy function is not coordinate invariant, as pointed out by Hill.[7] We present a simple version of his analysis and extend its scope. Consequential divergences in estimates of strength previously escaped notice since atomic bonds were at the same time differently modeled by the respective writers.

Whether convexity of the energy has a strong or a weak dependence on any reasonable choices of the geometric variables remains to be investigated; we intend in due course to make the appropriate calculations for at least one crystal model. Meanwhile, we are able here to use the published data themselves to show the qualitative divergences, with the help of some general comparison theorems.

Branching of a primary path of deformation, under a prescribed loading program, is well known to be closely associated with loss or exchange of stability. It follows that branching is likewise not coordinate invariant in general, when the criterion for its inception is stationarity of the conjugate forces during some virtual increment of deformation. On some paths, however, there are exceptional bifurcations that *are* substantially coordinate invariant on this criterion; we examine one such case in detail, in view of its possible role in any objective concept of ideal strength.

Finally, we treat thoroughly the loading of a cubic crystal by hydrostatic pressure or tension. This is an example of a natural environment where classical stability is not equivalent to convexity of the internal energy relative to *any* particular coordinates.

II. RELATIVITY OF STABILITY CRITERIA

Homogeneous pure strain of a crystal is specifiable by any six parameters that define the geometry of the primitive or other convenient cell. A natural set, chosen by Milstein,[4] is the lengths of the cell edges and their included angles. The squares and scalar products of the edge vectors form a set whose particular advantage resides in being elements of the metric tensor m_{ij}, relative to a reference configuration in which the cell is a unit cube. This specification, or the allied set of components e_{ij} of the Green's measure of strain, was always adopted by the Born school. No less convenient algebraically is the choice of Macmillan and Kelly,[3] namely, the elements of the stretch tensor λ_{ij} such that, if ξ_i and x_i are the reference and current rectangular coordinates of any lattice

vector, then

$$x_i = \lambda_{ij}\xi_j; \quad \lambda_{ij} = \lambda_{ji} \tag{1}$$

($i, j = 1, 2, 3$; summation convention). Expressed in these variables,

$$m_{ij} = \lambda_{ki}\lambda_{kj}, \tag{2}$$

$$e_{ij} = \tfrac{1}{2}(m_{ij} - \delta_{ij}), \tag{3}$$

where δ_{ij} is the Kronecker delta. In principle, disregarding possible complexities of analysis, one could use the components of any other measure of strain as generalized coordinates. Hill[7] considered any tensor coaxial with the principal fibers and having principal values $f(\lambda_1), f(\lambda_2), f(\lambda_3)$, where $\lambda_1, \lambda_2, \lambda_3$ are the principal stretches; $f(\lambda)$ can be any smooth monotone function such that $f(1) = 0$, $f'(1) = 1$ (normalizations that ensure coincidence with the classical infinitesimal strain when the deformation is first order). Simple examples of $f(\lambda)$ are $\lambda - 1$, $\ln\lambda$, $\frac{1}{2}(\lambda^2 - 1)$, the last of which generates the components of Eq. (3).

In conformity with the standard notation in Lagrangian mechanics, we denote an arbitrary set of generalized coordinates by $q_r, r = 1, \ldots, 6$. When, in particular, the geometric parameters are components of a tensor, say Green's strain, we put

$$q_1 = e_{11}, \quad q_2 = e_{22}, \quad q_3 = e_{33};$$

$$q_4 = 2e_{23}, \quad q_5 = 2e_{31}, \quad q_6 = 2e_{12}.$$

The internal energy, w per unit reference volume (i.e., w is the energy of the mass contained in the reference volume of the undeformed crystal), is supposed to be a determinate function of the set of q_r. The most widely used approximation has been to compute $2w$ by summing, over some 10^3 volume units of deformed crystal, the pairwise interaction energies associated with bonds on the representative atoms in one cell (the Lennard-Jones, or Born and Mayer, or Morse potentials are variously adopted). Metals whose electronic structures are not too complex have been modeled by adding a volume-dependent contribution to the interionic energies.[2] For our present concern, however, nothing need be assumed about the form or derivation of the function w.

As in classical mechanics, generalized conjugate variables are defined by

$$p_r = \frac{\partial w}{\partial q_r}, \quad r = 1, \ldots, 6. \tag{4}$$

The set of p_r can be related to the Cauchy tractions on the crystal (w being taken as the work of deformation per unit reference volume), but the connection is rarely simple. Analogously, in the continuum context, Hill[7] has introduced work-conjugate measures of stress, typically $t_{ij} = \partial w/\partial e_{ij}$, where e_{ij} stands for a strain tensor generated by any scale function $f(\lambda)$; w is, of course, symmetrized in the off-diagonal components and so $p_1 = t_{11}$, $p_2 = t_{22}$, $p_3 = t_{33}$, $p_4 = t_{23}$, $p_5 = t_{31}$, $p_6 = t_{12}$. Edifying interpretations of the conjugate stress tensors are available when (i) $f(\lambda) = \frac{1}{2}(\lambda^2 - 1)$ and (ii) $f(\lambda) = \lambda - 1$. For this purpose we fix attention on a cell that is a unit cube in the reference state and is subsequently subjected to a pure strain; the jth edge of the deformed cell is the vector with components λ_{kj} ($k = 1, 2, 3$). Let l_{ij} be the jth component of the load vector applied to the ith face of the cell; rotational balance of all loads requires that tensor $\lambda_{ik}l_{kj}$ be symmetric. Then in (i) the conjugate is such that $l_{ij} = t_{ik}\lambda_{kj}$ (which can be read as the decomposition of the ith load vector in terms of the triad of cell edges), while in (ii) the conjugate is simply $\frac{1}{2}(l_{ij} + l_{ji})$.

Elastic moduli are central in theories of branching and instability. We define a matrix of generalized moduli as the array of coefficients in the relations between differential increments of the conjugate sets of variables;

$$dp_r = c_{rs}dq_s, \quad c_{rs} = \frac{\partial^2 w}{\partial q_r \partial q_s} \tag{5}$$

($r, s = 1, \ldots, 6$; summation convention). The c_{rs} are of course dependent both on the level of strain and on the choice of generalized coordinates. However, when these are the elements of some strain measure, all such matrices coincide in the reference configuration itself, if it happens to be unstressed. In that case the c_{rs} are just conventional elastic moduli and the notation conforms with standard usage. In any deformed state we can now write the leading terms in a Taylor expansion of the internal energy in the alternative ways

$$\delta w = p_r\delta q_r + \tfrac{1}{2}c_{rs}\delta q_r\delta q_s + \cdots$$

$$= (p_r + \tfrac{1}{2}\delta p_r)\delta q_r + \cdots. \tag{6}$$

The latter can be viewed as an application of the trapezoid rule of quadrature.

To see how the moduli transform under a different choice of coordinates, let all new variables be distinguished by an asterisk and suppose each q_r is given as a function of the set of q_r^*. If the reference configuration also is changed, we have identically

$$p_u^* dq_u^*/\rho^* \equiv p_r dq_r/\rho$$

by invariance of the energy per unit mass of crystal, where ρ^* and ρ are the respective reference densities (i.e., the masses contained in the reference volumes). It follows that the conjugate variables transform according to

$$\frac{\rho}{\rho^*}p_u^* = \frac{\partial q_r}{\partial q_u^*}p_r . \tag{7}$$

Turning next to the moduli we take the differential of (7),

$$\frac{\rho}{\rho^*}dp_u^* = \frac{\partial q_r}{\partial q_u^*}dp_r + \frac{\partial^2 q_r}{\partial q_u^* \partial q_v^*}p_r\, dq_v^* ,$$

and substitute (5) and its asterisked analog. Comparison of the coefficients of the independent dq_v^* then gives

$$\frac{\rho}{\rho^*}c_{uv}^* = \frac{\partial q_r}{\partial q_u^*}\frac{\partial q_s}{\partial q_v^*}c_{rs} + \frac{\partial^2 q_r}{\partial q_u^* \partial q_v^*}p_r , \tag{8}$$

which is the transformation rule for the moduli. An equivalent calculation, starting from (6) and its asterisked analog, goes as follows:

$$\frac{1}{2}\left(\frac{1}{\rho^*}\delta p_u^* \delta q_u^* - \frac{1}{\rho}\delta p_r \delta q_r\right) = \left(\frac{1}{\rho}p_r \delta q_r - \frac{1}{\rho^*}p_u^* \delta q_u^*\right) + \cdots$$

$$= \frac{1}{\rho}p_r\left(\delta q_r - \frac{\partial q_r}{\partial q_u^*}\delta q_u^*\right) + \cdots ,$$

from (7). Whence

$$\frac{1}{\rho^*}\delta p_u^* \delta q_u^* - \frac{1}{\rho}\delta p_r \delta q_r = \frac{1}{\rho}p_r \frac{\partial^2 q_r}{\partial q_u^* \partial q_v^*}\delta q_u^* \delta q_v^* + \cdots , \tag{9}$$

from which we can recover (8) immediately. Also, the quadratic identity (9) will later be found useful in its own right. Moreover, its derivation makes evident a cardinal point: in transforming (6) the *linear* terms in the δq_r must for consistency be evaluated to *second* order in the new variables; indeed, it is precisely in these linear terms that the second partial derivatives in (8) originate.

We remark that these derivatives vanish automatically, however, when the transformation between two sets of generalized coordinates is strictly linear. This happens, for example, when the two are simply equivalent representations of some tensor measure of strain on different bases in a fixed reference state; in that case (8) becomes an expression of the transformation rule for a fourth-rank tensor. The second derivatives also vanish when the generalized coordinates are the molar parameters and the reference state itself is changed; for, if λ_{ij}^0 is the fixed stretch from state ρ to state ρ^*, we have $\lambda_{ij} = \lambda_{ki}^* \lambda_{kj}^0$ via Eq. (1), and so $m_{ij} = \lambda_{ki}^0 \lambda_{lj}^0 m_{kl}^*$. By Eq. (3) the corresponding transformation between the respective sets of Green's variables is likewise linear (though not homogeneous).

Coming, now, to stability, we take this to signify that the combined incremental potential energy of the crystal and its external loading is positive for small arbitrary variations of the chosen set of q_r. This accords with the classical definition; it is tacitly assumed not only that the loads are conservative but that their virtual work is a function of the q_r alone. Plainly, this entails the notion of ideal strength as an *intrinsic* property of the material. By contrast, the loading in laboratory experiments is usually frame dependent and the work is affected also by rotation of the specimen (cf. Hill's[7] analysis of dead loading, in particular). On the intrinsic view, the loads "follow" the material during any disturbance; they may, in addition, be deformation sensitive and so become different in kind from those in the state of equilibrium whose stability is under test. In any event, the increment δu of external work must be specified objectively to second order, like the increment δw of internal energy, and is expressible as

$$\delta u = p_r \delta q_r + \tfrac{1}{2}k_{rs}\delta q_r \delta q_s + \cdots \tag{10}$$

per unit reference volume, where the coefficients k_{rs} depend on the test configuration and the choice of variables. The linear terms are necessarily the same as in Eq. (6) since the combined potential energy is stationary when all $\delta q_r = 0$. In a disturbed configuration the *virtual* state of stress that would be in *statical balance* with the follower loads is represented by values $p_r + k_{rs}\delta q_s$ of the conjugate forces. The *actual* state of stress is, of course, represented by values $p_r + c_{rs}\delta q_s$.

Under change of variables the invariance of $\delta u/\rho$ requires that the symmetrized k_{rs} transform according to

$$\frac{\rho}{\rho^*}k_{uv}^* = \frac{\partial q_r}{\partial q_u^*}\frac{\partial q_s}{\partial q_v^*}k_{rs} + \frac{\partial^2 q_r}{\partial q_u^* \partial q_v^*}p_r , \tag{11}$$

in analogy with (8). The algebraic expression of the stability criterion, namely,

$$(c_{rs} - k_{rs})\delta q_r \delta q_s > 0 , \quad \text{when not all } \delta q_r = 0 , \tag{12}$$

is of course coordinate invariant. In verification,

$$\frac{\rho}{\rho^*}(c_{uv}^* - k_{uv}^*) = \frac{\partial q_r}{\partial q_u^*}\frac{\partial q_s}{\partial q_v^*}(c_{rs} - k_{rs})$$

from (8) and (11), and so

$$(1/\rho^*)(c_{uv}^* - k_{uv}^*)\delta q_u^* \delta q_v^* = (1/\rho)(c_{rs} - k_{rs})\delta q_r \delta q_s .$$

Writers on crystal strength have customarily retained only the linear terms in the incremental work [Eq. (10)]. Thus, the criterion has been routinely expressed as

$$c_{rs}\delta q_r \delta q_s = \frac{\partial^2 w}{\partial q_r \partial q_s}\delta q_r \delta q_s > 0 , \tag{13}$$

regardless of the choice of variables. The inequality can be described as requiring that w be locally strictly convex in its arguments, or that the Hessian matrix of w be positive definite. That the criterion (13) is generally not coordinate invariant

is already evident from the previous analysis. We can make it explicit by means of the exact connection (8) or by reproducing the second-degree terms in series (9):

$$\frac{\rho}{\rho^*}c^*_{uv}\delta q^*_u\delta q^*_v - c_{rs}\delta q_r\delta q_s = p_r\frac{\partial^2 q_r}{\partial q^*_u\partial q^*_v}\delta q^*_u\delta q^*_v\,. \tag{14}$$

Cases have already been instanced when the right-hand side vanishes here; otherwise its sign is uncertain *a priori* and at this stage the local convexity of w^* remains in doubt. We proceed to examine the matter in more detail for the sets of coordinates principally favored in the literature.

III. COMPARISON THEOREMS

Without losing generality we can suppose that in some reference configuration the representative cell is a cube and that its edge is adopted as the unit of length. We examine the divergent predictions of the convexity criterion relative to three sets of generalized coordinates referred to this basis: the edges and angles of the deformed cell (Milstein); the components of the Green's tensor (Born); and the components of the stretch tensor (Macmillan and Kelly[8]).

Denote the coordinates corresponding to the basis components of the Green's tensor [Eq. (3)] by $q_1, \ldots, q_6$ and those corresponding to the stretch tensor [Eq. (1)] by $q_1^*, \ldots, q_6^*$. The connections [Eq. (2)] give

$$2q_1 = q_1^{*2} + \tfrac{1}{4}q_5^{*2} + \tfrac{1}{4}q_6^{*2} - 1\,,\quad 2q_4 = (q_2^* + q_3^*)q_4^* + \tfrac{1}{2}q_5^*q_6^*\,,$$

etc. Calculation of the right-hand side in (14) leads quickly to

$$\begin{aligned} S - G = {} & t_{11}[(\delta\lambda_{11})^2 + (\delta\lambda_{12})^2 + (\delta\lambda_{13})^2] + \cdots + \cdots \\ & + 2t_{23}[(\delta\lambda_{22} + \delta\lambda_{33})\delta\lambda_{23} + \delta\lambda_{12}\delta\lambda_{13}] + \cdots + \cdots\,, \end{aligned} \tag{15}$$

where S and G are mnemonic symbols for the Hessian forms in the stretch and Green's variables, respectively, and tensor t_{ij} is the work conjugate of the Green's measure (its physical interpretation was given earlier).

Next, with $q_1, \ldots, q_6$ retaining their meanings but q_1^*, q_2^*, q_3^* denoting the edges of the deformed cell and q_4^*, q_5^*, q_6^* their included angles, we have

$$2q_1 = q_1^{*2} - 1\,,\quad q_4 = q_2^*q_3^*\cos q_4^*\,,$$

etc. For simplicity suppose that the path of deformation is such that the cell becomes rectangular with edges $\lambda_1, \lambda_2, \lambda_3$. After an arbitrary incremental deformation the cell becomes a parallelepiped and its edges are no longer the principal fibers of the total deformation. One may show by elementary geometry that

$$\delta q_1^* = \delta\lambda_1 = \delta\lambda_{11}\,,\quad \delta q_4^* = -[(\lambda_2 + \lambda_3)/\lambda_2\lambda_3]\delta\lambda_{23}\,,$$

etc., to first order, where the stretches of the new principal fibers are denoted by $\lambda_1 + \delta\lambda_1$, etc. After carrying out the differentiations in (14) we set $q_4^* = q_5^* = q_6^* = \frac{1}{2}\pi$, and recast the result in the stretch variables:

$$\begin{aligned} M - G = {} & t_{11}(\delta\lambda_1)^2 + \cdots + \cdots \\ & + 2t_{23}(\lambda_2 + \lambda_3)\delta\ln(\lambda_2\lambda_3)\delta\lambda_{23} + \cdots + \cdots\,, \end{aligned} \tag{16}$$

where M stands for the Hessian form in the Milstein variables.

In the literature, most stability computations under load are for initially cubic crystals which are deformed so that the symmetry becomes orthorhombic with respect to the principal fibers. We choose a representative cell with edges parallel to these symmetry axes. Its faces are then subject to purely normal loads, say l_1, l_2, l_3, and the shearing stresses vanish in (15) and (16). These accordingly reduce to

$$S - G = (l_1/\lambda_1)[(\delta\lambda_1)^2 + (\delta\lambda_{12})^2 + (\delta\lambda_{13})^2] + \cdots + \cdots\,, \tag{17}$$

$$M - G = \frac{l_1}{\lambda_1}(\delta\lambda_1)^2 + \frac{l_2}{\lambda_2}(\delta\lambda_2)^2 + \frac{l_3}{\lambda_3}(\delta\lambda_3)^2\,, \tag{18}$$

which together yield

$$S - M = (l_1/\lambda_1)[(\delta\lambda_{12})^2 + (\delta\lambda_{13})^2] + \cdots + \cdots\,. \tag{19}$$

These simple connections enable the predictions of stability via the respective convexity criteria to be directly compared. We instance some typical applications in the specific contexts of the published data.

We begin with a general observation. When the principal loads are all non-negative, so are the forms $S - G$, $M - G$, and $S - M$, allowing the one-way implications:

G stable $\rightarrow$ M stable $\rightarrow$ S stable, when $l_1, l_2, l_3 \geq 0$;

similarly,

S stable $\rightarrow$ M stable $\rightarrow$ G stable, when $l_1, l_2, l_3 \leq 0$.

In these the prefix indicates, on the present view, that the particular Hessian is positive definite. On a path of deformation leading from a stable, unstressed, reference configuration (where every Hessian is positive definite) the estimated onsets of failure may be correspondingly ordered:

$$G \text{ strength} \leq M \text{ strength} \leq S \text{ strength}, \quad \text{when } l_1, l_2, l_3 \geq 0\,; \tag{20}$$

$$S \text{ strength} \leq M \text{ strength} \leq G \text{ strength}, \quad \text{when } l_1, l_2, l_3 \leq 0\,. \tag{21}$$

In this context "failure" means that a specific Hessian becomes semidefinite, while "strength" denotes the associated stage of deformation (rather than the load magnitude). To extract more information, we must attend to the critical variation $\delta\lambda_{ij}$ that causes a semidefinite Hessian to vanish (and which *ipso facto* renders it stationary in the class of arbitrary variations). Suppose, for example, in (20) that the G critical $\delta\lambda_{ij}$ simultaneously makes $M-G$ vanish; then the G and M strengths coincide. If, on the other hand, $M>G$ for that $\delta\lambda_{ij}$, the first inequality in (20) is strict. An analogous statement can be made for every like-ordered pair in (20) and (21).

In the pioneering investigation by Born and Fürth[9] an initially face-centered-cubic lattice was loaded uniaxially in a cubic direction ($l_1\neq 0$, $l_2=l_3=0$). A Lennard-Jones model was adopted and the G strengths were computed for both tension and compression. In neither case was the critical variation described explicitly; we infer with hindsight that in tension it would be $\delta\lambda_1=0$, $\delta\lambda_2=-\delta\lambda_3\neq 0$, coaxial with the basis, while in compression it would be the *actual* $\delta\lambda_{ij}$ at the algebraic minimum of the Green's conjugate stress l_1/λ_1.[10] The critical variation in tension is such that $S=M=G=0$, while in compression it is such that $S=M<G=0$. For Born and Fürth's crystal, therefore, it may be concluded that in tension the three strengths are equal, but that in compression the G strength is the greatest.

We turn, next, to the computations of Macmillan and Kelly[3] for the S strengths of sodium chloride (Born-Mayer model) and argon (Lennard-Jones model). The reference basis and configuration are the cubic axes of the experimentally observed (and theoretically stable) structures at zero stress and temperature. Three paths of deformation are followed: (i) uniaxial extension with $\lambda_1>1$, $\lambda_2=\lambda_3=1$; (ii) uniaxial tension with $l_1>0$, $l_2=l_3=0$; (iii) plane dilatation with $\lambda_1=1$, $\lambda_2=\lambda_3>1$. All three loads remain tensile along the path segments (i) and (iii), and consequently (20) applies in every case. For sodium chloride Macmillan and Kelly found the critical variation to be (i), such as would actually occur under a *uniaxial* load increment $\delta l_1\neq 0$, $\delta l_2=\delta l_3=0$ (the stage in question being prior to the path maximum of l_1); (ii) the actual $\delta\lambda_{ij}$ at maximum l_1; (iii) $\delta\lambda_1=0$, $\delta\lambda_2=-\delta\lambda_3\neq 0$, coaxial with the basis. For argon Macmillan and Kelly did not report (i), while the critical variation in (ii) was $\delta\lambda_1=0$, $\delta\lambda_2=-\delta\lambda_3\neq 0$, coaxial with the basis, and in (iii) was $\delta\lambda_1/\delta\lambda_2\simeq -\frac{7}{5}$, $\delta\lambda_2=\delta\lambda_3$, coaxial with the basis. Thus the critical variations in (i), (ii), and (iii) for sodium chloride and in (iii) for argon are such that $G<M=S=0$; we conclude that in all these cases the G strength is certainly less than the S strength, but we cannot otherwise sharpen (20). The critical variation in (ii) for argon is such that $G=M=S=0$ and so again (20) cannot be sharpened.

As our final illustration we cite some work by Milstein on uniaxial loading of iron[4] (Morse model) and nickel[5] (generalized Morse model). For iron, the stable unstressed reference configuration was body-centered cubic. Under tension the critical variation was the actual $\delta\lambda_{ij}$ at maximum load, making $G<S=M=0$; under compression it was $\delta\lambda_1=0$, $\delta\lambda_2=-\delta\lambda_3\neq 0$, coaxial with the basis, making $G=S=M=0$. We conclude that in tension the S strength is equal to the M strength, which exceeds the G strength, while in compression the G and M strengths are equal. For nickel, the stable unstressed reference configuration was face-centered cubic. Under tension the critical variation was $\delta\lambda_1=0$, $\delta\lambda_2=-\delta\lambda_3\neq 0$, coaxial with the basis, making $G=S=M=0$; under compression it was the actual $\delta\lambda_{ij}$ at the algebraically minimum load, making $G>S=M=0$. We conclude that in tension the S strength is equal to the M strength, while in compression the G strength exceeds the M strength.

IV. BIFURCATIONS

We return to the stability criterion for the general case where the external work involves k_{rs} terms as in Eq. (10), when expressed in the chosen variables. On a path issuing from a stable state the criterion [Eq. (12)] is either perpetually satisfied, or a stage is reached when the quadratic form is momentarily semidefinite (and thereafter indefinite along some further segment). At this critical stage the homogeneous equations

$$\delta p_r - k_{rs}\delta q_s = 0 \tag{22}$$

necessarily have at least one eigensolution which causes the quadratic to vanish. This set of equations is, of course, form invariant under transformation, as can be verified readily from Eqs. (7) and (11), or from the formula following (12).

Changing the viewpoint, at each stage of the path we could propose the following question: If the values of the Pfaffians $dp_r - k_{rs}dq_s$, $r=1,\ldots,6$, are prescribed in a further active loading of the crystal, are the increments dq_r in the generalized coordinates uniquely determined? Obviously, the answer is affirmative when (22) has only a null solution. At the critical stage, on the other hand, the coordinate increments are nonunique to the extent of arbitrary additive multiples of each eigendeformation under passive loading (the same could be said at any subsequent stage where the quadratic (12) is again stationary, even though not

semidefinite). In this sense the loss of stability on the primary path is associated with a possible bifurcation, wherein more than one mode of deformation corresponds to given Pfaffians. By analogy with standard branching theory for discrete mechanical systems, the starting direction of a secondary path is decided by a higher-order specification of the post-critical loading program; we do not pursue that aspect here, while recognizing its likely relevance to a satisfactory account of "ideal strength."

Instead, we go a little more deeply into the first-order theory. Suppose that crystal stability is tested in an environment where the external work δu is such that the k_{rs} terms in (10) can be removed by appropriately choosing the coordinates. Then the corresponding eigenequations are

$$\delta p_r = c_{rs}\delta q_s = 0\,, \tag{23}$$

in parallel with (13), and the passive loading induced by any such δq_s renders all conjugate variables stationary. We can express this in another way by noting that dp_s associated with any dq_r at the critical stage has the property

$$dp_s\delta q_s = (c_{sr}dq_r)\delta q_s = (c_{sr}\delta q_s)dq_r = 0 \tag{24}$$

since $c_{rs} = c_{sr}$. The interpretation is that the modulus which, in a generalized sense, governs incremental deformation of type δq_s vanishes when $\det(c_{rs}) = 0$.[11]

With premise (23) we search for bifurcations on a path of deformation through an unstressed cubic configuration of the crystal lattice. With the cubic cell as reference basis we suppose coordinates assigned so that q_4, q_5, q_6 remain fixed and equal when the cell stays rectangular, while generally each of the groups q_1, q_2, q_3 and q_4, q_5, q_6 accord equal weightings to the three cubic directions. Among such choices are the stretch variables, the Milstein parameters, and any of the Hill measures of strain. For the primary path we take axisymmetric deformation, $\lambda_2 = \lambda_3$, under uniaxial loading $l_1 \neq 0$, $l_2 = l_3 = 0$; correspondingly, only the conjugate variable p_1 is nonzero. Along this path the crystal symmetry remains at least tetragonal. The differential relations [Eq. (5)], governing an arbitrary disturbance, consequently reduce to

$$\begin{aligned} dp_1 &= c_{11}dq_1 + c_{12}(dq_2 + dq_3)\,,\\ dp_2 &= c_{12}dq_1 + c_{22}dq_2 + c_{23}dq_3\,,\\ dp_3 &= c_{12}dq_1 + c_{23}dq_2 + c_{22}dq_3\,; \end{aligned} \tag{25}$$

$$dp_4 = c_{44}dq_4\,,\quad dp_5 = c_{55}dq_5\,,\quad dp_6 = c_{55}dq_6\,. \tag{26}$$

We have here incorporated the lattice symmetries

$$c_{12} = c_{13}\,,\quad c_{22} = c_{33}\,,\quad c_{55} = c_{66}\,,$$

as well as the conjugacy symmetries $c_{rs} = c_{sr}$. Then

$$\det(c_{rs}) = (c_{22} - c_{23})[c_{11}(c_{22} + c_{23}) - 2c_{12}^2]c_{44}c_{55}^2\,, \tag{27}$$

showing that the leading 3×3 minor factorizes. Necessary and sufficient conditions for stability, as judged by the requirement (13) for positive definite c_{rs}, are

$$c_{11} > 0\,,\quad c_{22} + c_{23} > 2c_{12}^2/c_{11}\,,\quad c_{22} - c_{23} > 0 \tag{28}$$

together with

$$c_{44} > 0\,,\quad c_{55} > 0\,. \tag{29}$$

This set of inequalities is preferred to other equivalents because it involves the determinantal factors directly. The corresponding reduction of $c_{rs}\delta q_r\delta q_s$ to a sum of independent squares (not the canonical normal form, however) is

$$\begin{aligned} &[c_{11}\delta q_1 + c_{12}(\delta q_2 + \delta q_3)]^2/c_{11}\\ &\quad + \tfrac{1}{2}(c_{22} + c_{23} - 2c_{12}^2/c_{11})(\delta q_2 + \delta q_3)^2\\ &\quad + \tfrac{1}{2}(c_{22} - c_{23})(\delta q_2 - \delta q_3)^2\\ &\quad + c_{44}\delta q_4^2 + c_{55}(\delta q_5^2 + \delta q_6^2)\,. \end{aligned} \tag{30}$$

The determinant can vanish when, and only when, at least one factor does. Each vanishing factor is associated with a particular type of eigensolution; apart from arbitrary multipliers, the types are

$$\begin{aligned} &(2c_{12}, -c_{11}, -c_{11}, 0, 0, 0),\quad \text{when } c_{22} + c_{23} = 2c_{12}^2/c_{11}\,,\\ &(0, 1, -1, 0, 0, 0),\quad \text{when } c_{22} - c_{23} = 0\,,\\ &(0, 0, 0, 1, 0, 0),\quad \text{when } c_{44} = 0\,,\\ &(0, 0, 0, 0, 1, 0) \text{ and } (0, 0, 0, 0, 0, 1),\quad \text{when } c_{55} = 0\,, \end{aligned} \tag{31}$$

as may be verified by substitution in (25) and (26), or as is self-evident from (30). We have thereby proved that these are the only possible eigensolutions; the first two types were encountered, as we have already mentioned, in numerical computations by Macmillan and Kelly[3] and by Milstein[4,5] with particular sets of coordinates.

In each case in (31) the eigenstate terminates a *stable* range of deformation when the four remaining inequalities in (28) and (29) stand, so that (30) is positive semidefinite. Otherwise an eigenstate is embedded in an unstable range where (30) is indefinite or negative definite.

On the presently considered primary path the coordinate increments at any stage are

$$(c_{22} + c_{23}, -c_{12}, -c_{12}, 0, 0, 0)[c_{11}(c_{22} + c_{23}) - 2c_{12}^2]^{-1}dp_1 \tag{32}$$

from (25). We see, therefore, that the first kind of eigenstate in (31) occurs where the conjugate

variable p_1 passes through a stationary value, so that the associated Young's modulus vanishes; moreover, the eigensolution is just the path increment itself. Stationarity of p_1 is, of course, not coordinate invariant. For example, p_1 for either the stretch or Milstein variables is the applied load l_1, while p_1 for the Green's variables is l_1/λ_1 (an edge of the reference cell being taken, as usual, to be the unit of length). We can view this relativity also from the standpoint of the generalized moduli. Thus, if for the moment c_{rs} denotes the Green's moduli and c^*_{rs} the Milstein moduli, it can be shown from (8) that

$$c^*_{11} = \lambda_1^2 c_{11} + l_1/\lambda_1\,, \quad c^*_{22} = \lambda_2^2 c_{22}\,, \quad c^*_{12} = \lambda_1\lambda_2 c_{12}\,,$$
$$c^*_{23} = \lambda_2^2 c_{23}\,, \quad c^*_{44} = \lambda_2^4 c_{44}\,, \quad c^*_{55} = \lambda_1^2\lambda_2^2 c_{55} \tag{33}$$

on the primary path. Evidently the condition for the first type of eigenstate in (31) is not attained simultaneously by both sets of variables. Similar formulae also relate the stretch moduli to the Green's moduli, except that the final two entries are replaced by $\lambda_2^2 c_{44}$ and $\frac{1}{4}(\lambda_1+\lambda_2)^2 c_{55} + \frac{1}{4}p_1$, respectively, on the primary path.

By contrast, the condition (31) for the second type of eigenstate *is* invariant, together with the eigensolution. To show this, we observe first from (11) that the premise $k_{rs} = 0$ implies

$$k^*_{uv} = p_1 \frac{\partial^2 q_1}{\partial q^*_u \partial q^*_v}$$

for any other variables and the same reference basis. Furthermore, in the presumed eigenstate where $c_{22} = c_{23}$, the solution $\delta q_r \propto (0, 1, -1, 0, 0, 0)$ is represented by

$$\delta q^*_u = \frac{\partial q^*_u}{\partial q_r}\delta q_r \propto \left(\frac{\partial}{\partial q_2} - \frac{\partial}{\partial q_3}\right) q^*_u$$

in any asterisked coordinates. But the primary path is endowed with the symmetries

$$\left(\frac{\partial}{\partial q_2} - \frac{\partial}{\partial q_3}\right)(q^*_1, q^*_4, q^*_5, q^*_6) = 0\,,$$

$$\left(\frac{\partial}{\partial q_2}, \frac{\partial}{\partial q_3}\right) q^*_2 = \left(\frac{\partial}{\partial q_3}, \frac{\partial}{\partial q_2}\right) q^*_3\,,$$

within the assigned class of coordinate choices, and consequently $\delta q^*_u \propto (0, 1, -1, 0, 0, 0)$. Therefore,

$$k^*_{uv}\delta q^*_v \propto k^*_{u2} - k^*_{u3} = p_1\left(\frac{\partial}{\partial q^*_2} - \frac{\partial}{\partial q^*_3}\right)\frac{\partial q_1}{\partial q^*_u} = 0$$

on the primary path, by like symmetries. Hence $\delta p^*_u = 0$ by (22) since that equation is form invariant. Equivalently, $c^*_{uv}\delta q^*_v = 0$ which implies that $c^*_{22} = c^*_{23}$; this condition can also be verified directly from (8), in conjunction with the symmetries just listed. In summary, the routine omission of the second-order terms in the external work (10), irrespective of the choice of coordinates, does not in this case lead to divergent predictions of either the eigensolution or the eigenstate. (We remark, however, that it is another matter whether stability is always judged to be *first* lost there or not.) The actual eigendeformation represented invariantly by $(0, 1, -1, 0, 0, 0)$ can be identified readily from any convenient choice of coordinates: it is an incremental pure shear at 45° to the reference axes in the 2-3 plane [i.e., in the plane of Miller indices $(0, 1, 1)$]. As to the load environment in a test of stability, we might, for instance, envisage that this is such that every $k_{rs} = 0$ when the external work is expressed in the Green's variables. Then, during any disturbance, the load vector on each face of the deformed cell varies passively as if it were a fiber embedded in the material.[7] In particular, the uniaxial load would remain *dead* during the incremental shear. Therefore, this eigendeformation for the envisaged criterion of stability is similar in type to the branching strain increment on an intersecting *secondary* path along which $q_2 \neq q_3$ under uniaxial load. That an incipient bifurcation $dq_r \propto (0, 1, -1, 0, 0, 0)$ is initiated under stationary load when $c_{22} = c_{23}$ is, of course, also directly apparent from (25) and (26) written in the Milstein variables.

We come, finally, to the third and fourth types of eigenstate in (31). With any reasonable choice of coordinates, the $(0, 0, 0, 1, 0, 0)$ eigensolution represents a shear parallel to the reference axes in the 2-3 plane. It is seen in calculations for iron,[4] relative to the Milstein variables and a cubic reference cell in the unstressed body-centered configuration, where it terminates the associated stable range on the tension side [as judged by (28) and (29) in these variables]. The $(0, 0, 0, 1, 0, 0)$ eigensolution is seen also in calculations for nickel,[5] relative to the Milstein variables and a cubic reference cell in the unstressed face-centered configuration. However, in that case, the eigenstate is embedded in an unstable range on the compression side, beyond the algebraic minimum in the load.

With these Morse models, or whenever the strain energy comes solely from pairwise interactions, it is known[7] that the Green's moduli possess the Cauchy symmetries

$$c_{44} = c_{23}\,, \quad c_{55} = c_{12}\,.$$

Correspondingly, from (33), the Milstein moduli on the considered primary path are such that

$$c^*_{44} = \lambda_2^2 c^*_{23}\,, \quad c^*_{55} = \lambda_1\lambda_2 c^*_{12}\,,$$

as can be recognized also from explicit lattice

summations for the moduli.[4] Thus c_{23}^* or c_{12}^* vanish with c_{44}^* or c_{55}^*, respectively. The latter characterizes the fourth type of eigenstate in (31), which is observed for both iron and nickel when loaded in tension from their unstressed face-centered configurations. However, these eigenstates are embedded in unstable ranges, namely where $c_{44}^* < 0$ for iron and where $c_{22}^* - c_{23}^* < 0$ for nickel.

V. STABILITY OF PURE VOLUMETRIC DEFORMATION

A well-defined loading environment, which is also technically uncomplicated, is provided by a uniformly pressurized fluid. We suppose the apparatus designed so that the pressure on the crystal does not vary during any departure from a primary configuration of equilibrium. Plainly, this passive loading is conservative and its external work δu during a δ departure is just the pressure p times the further decrease in volume. The latter is conveniently calculated with the Milstein variables: if the reference cell when arbitrarily deformed has edges a, b, c and included angles α, β, γ, its volume is

$$abc(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)^{1/2} .$$

Assuming that the unstressed lattice is cubic, the deformation on the primary path is purely volumetric. The edges of the reference cell are equal to the all-round stretch λ, and so with $a = \lambda + \delta a$ and $\alpha = \frac{1}{2}\pi + \delta\alpha$, etc., in a disturbed configuration

$$\delta u/p\lambda = -\lambda(\delta a + \delta b + \delta c) - (\delta a\delta b + \delta b\delta c + \delta c\delta a) + \tfrac{1}{2}[(\lambda\delta\alpha)^2 + (\lambda\delta\beta)^2 + (\lambda\delta\gamma)^2] + \cdots , \quad (34)$$

to second order in the δ variations. By comparison with (10) we can read off the coefficients

$$k_{11}^M = 0 , \quad k_{12}^M = -p\lambda , \quad k_{44}^M = p\lambda^3 \quad (35)$$

relative to the Milstein variables. The corresponding coefficients for the Green's and stretch variables are

$$\begin{aligned} &k_{11}^G = p/\lambda , \quad k_{12}^G = -p/\lambda , \quad k_{44}^G = p/\lambda ; \\ &k_{11}^S = 0 , \quad k_{12}^S = -p\lambda , \quad k_{44}^S = \tfrac{1}{2}p\lambda . \end{aligned} \quad (36)$$

These values can be derived from the transformation equations (11) in conjunction with (35); or more simply from (15) and (16) specialized to pressure loading, with M, G, and S there standing now for the respective forms $k_{rs}\delta q_r\delta q_s$ (instead of $c_{rs}\delta q_r\delta q_s$).

On the primary path the Hessian form in any variables can be arranged as

$$\begin{aligned} c_{rs}\delta q_r\delta q_s = {} & \tfrac{1}{3}(c_{11} + 2c_{12})(\delta q_1 + \delta q_2 + \delta q_3)^2 \\ & + \tfrac{1}{3}(c_{11} - c_{12})[(\delta q_1 - \delta q_2)^2 + \cdots + \cdots] \\ & + c_{44}[(\delta q_4)^2 + (\delta q_5)^2 + (\delta q_6)^2] . \end{aligned} \quad (37)$$

When the environment also has cubic symmetry, the form $k_{rs}\delta q_r\delta q_s$ can be expanded similarly. The stability criterion (12) then yields the conditions

$$\begin{aligned} &c_{11} + 2c_{12} > k_{11} + 2k_{12} , \\ &c_{11} - c_{12} > k_{11} - k_{12} , \\ &c_{44} > k_{44} , \end{aligned} \quad (38)$$

which are of course coordinate invariant as in (12). For example, this may be verified for the Milstein, Green's, and stretch variables from (35), (36), and the connections

$$\begin{aligned} &\lambda^2 c_{11}^G = c_{11}^M + p\lambda , \quad \lambda^2 c_{12}^G = c_{12}^M , \quad \lambda^4 c_{44}^G = c_{44}^M ; \\ &c_{11}^S = c_{11}^M , \quad c_{12}^S = c_{12}^M , \quad \lambda^2 c_{44}^S = c_{44}^M - \tfrac{1}{2}p\lambda^3 ; \end{aligned} \quad (39)$$

which follow from (8).

In fact, every set of conditions (38) is equivalent to

$$\kappa > 0 , \quad \mu > 0 , \quad \mu' > 0 , \quad (40)$$

where κ is the ordinary bulk modulus, $-\frac{1}{3}\lambda dp/d\lambda$, while μ and μ' are the usual shear moduli in the relations between the cubic-axes components of the Cauchy stress increment $\delta\sigma_{ij}$ and the rotationless strain increment $\delta\epsilon_{ij}$ (reckoned conventionally, relative to the *current* configuration). To establish this equivalence we observe first that, for the current cell volume λ^3,

$$2(\delta w - \delta u) = \lambda^3\delta\sigma_{ij}\delta\epsilon_{ij} + \cdots \quad (41)$$

to second order, where δu is given by (34) and summation is implied over $i, j = 1, 2, 3$. The right-hand term comes from the *varying* part of the actual Cauchy stress, $-p\delta_{ij} + \delta\sigma_{ij}$, in the crystal after a further deformation $\delta\epsilon_{ij}$; the second-order effects of the interaction between $-p\delta_{ij}$ itself and $\delta\epsilon_{ij}$ are already fully accounted for in δu. Analogously to (37) we have, from first principles in strain geometry,

$$\begin{aligned} \lambda^2\delta\sigma_{ij}\delta\epsilon_{ij} = {} & \kappa(\delta a + \delta b + \delta c)^2 + \tfrac{2}{3}\mu[(\delta a - \delta b)^2 + \cdots + \cdots] \\ & + \mu'[(\lambda\delta\alpha)^2 + (\lambda\delta\beta)^2 + (\lambda\delta\gamma)^2] \end{aligned} \quad (42)$$

expressed in the Milstein variables. Conditions (40) now follow at once from the classical stability criterion, which requires (41) and hence (42) to be positive definite. Next, with $2(\delta w - \delta u)$ given by (12) in these same variables, we can compare coefficients on both sides of (41):

$$\begin{aligned} &(c_{11}^M + 2c_{12}^M) - (k_{11}^M + 2k_{12}^M) = 3\kappa\lambda , \\ &(c_{11}^M - c_{12}^M) - (k_{11}^M - k_{12}^M) = 2\mu\lambda , \\ &c_{44}^M - k_{44}^M = \mu'\lambda^3 . \end{aligned} \quad (43)$$

The detailed equivalence between (38) and (40) is now apparent. Finally, by combining (35) and (43), the Milstein moduli are obtained as

$$c_{11}^{M}=(\kappa+\tfrac{4}{3}\mu)\lambda\,,\quad c_{12}^{M}=(\kappa-\tfrac{2}{3}\mu-p)\lambda\,,\quad c_{44}^{M}=(\mu'+p)\lambda^{3} \tag{44}$$

in terms of κ, μ, μ' and the function $p(\lambda)$ on the primary path. The moduli relative to any other variables follow by applying (8), as in the derivation of (39) for the Green's and stretch moduli.

Possible eigenstates under pressure loading make (42) semidefinite, and the critical variations are evidently of the following types:

$$\begin{aligned}&(1,1,1,0,0,0)\delta\lambda\,,\quad \text{when } \kappa=0\,;\\ &(\delta a,\delta b,\delta c,0,0,0) \text{ with } \delta a+\delta b+\delta c=0\,,\\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{when } \mu=0\,;\\ &(0,0,0,\delta\alpha,\delta\beta,\delta\gamma)\,,\quad \text{when } \mu'=0\,.\end{aligned} \tag{45}$$

In the first type the eigendeformation is purely volumetric and is just the actual increment on the primary path where p is stationary. For actual crystals this would normally be expected only under hydrostatic tension, namely where p passes through a negative minimum. Computations of the $p(\lambda)$ relation for various model lattices agree with this expectation. For example, Milstein[12,13] found that for Morse function and generalized Morse function calculations, κ decreases with increasing λ but remains positive while $\lambda<1$, and Macmillan and Kelly[14] found that κ vanishes for argon (Lennard-Jones model) when $\lambda=1.09$ and for sodium chloride (Born-Mayer model) when $\lambda=1.16$. The second type of eigendeformation makes the cell orthorhombic at constant volume; the third type changes the included angles independently but preserves the edge lengths. We are not aware of any data on the stretch dependences of μ and μ'. It might be instructive to investigate for some model lattice the mutual ordering of the three eigenstates.

Stability on the primary path might alternatively be judged by convexity of the internal energy function, relative to some set of generalized coordinates. This, as we have explained, is tantamount to postulating a passive loading environment such that all coefficients k_{rs} are zero at any stage on the path. It seems that the "natural" environment for pure volumetric deformation does not admit such coordinates; to that extent, therefore, the convexity criterion in this context appears as an entirely notional concept of crystal strength. Whether or not this is a correct assessment, we think it worthwhile to set down the implications, in order to give further emphasis to our main thesis.

By reference to (37) or (38), the convexity conditions for stability are

$$c_{11}+2c_{12}>0\,,\quad c_{11}-c_{12}>0\,,\quad c_{44}>0\,, \tag{46}$$

relative to the choice of generalized coordinates. The eigenstates and critical variations, under which the conjugate forces are stationary, are

$$\begin{aligned}&(1,1,1,0,0,0)\,,\quad \text{when } c_{11}+2c_{12}=0\,;\\ &(\delta q_1,\delta q_2,\delta q_3,0,0,0)\,,\quad \text{with } \delta q_1+\delta q_2+\delta q_3=0\,,\\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{when } c_{11}-c_{12}=0\,;\\ &(0,0,0,\delta q_4,\delta q_5,\delta q_6)\,,\quad \text{when } c_{44}=0\,.\end{aligned} \tag{47}$$

With the Green's, Milstein, and stretch variables in turn as generalized coordinates, the predictions of (46) with (39) and (44) are as follows:

$$\begin{aligned}&G \text{ stable}:\ \kappa>\tfrac{1}{3}p\,,\quad \mu>-p\,,\quad \mu'>-p\,;\\ &M \text{ stable}:\ \kappa>\tfrac{2}{3}p\,,\quad \mu>-\tfrac{1}{2}p\,,\quad \mu'>-p\,;\\ &S \text{ stable}:\ \kappa>\tfrac{2}{3}p\,,\quad \mu>-\tfrac{1}{2}p\,,\quad \mu'>-\tfrac{1}{2}p\,.\end{aligned} \tag{48}$$

Where such stable ranges of deformation have finite limits, these accord with the ordering in (20) when $p<0$, and in (21) when $p>0$. This may, for example, be seen from qualitative sketches of any single-valued dependences of p, μ, and μ' on λ, remembering that $\kappa=-\frac{1}{3}\lambda\,dp/d\lambda$. With the expected $p(\lambda)$ relation, and speaking only of the first type of eigendeformation, the ranges of M and S stability are identical and exceed the G range, which itself extends beyond the point where the bulk modulus vanishes.

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[11]The vanishing of a certain determinant is the arbitrary *starting point* in Basinski *et al.*'s[2] computations of ideal strength. It appears that the elements in their determinant are the coefficients in the relations between the Jaumann derivative of Cauchy stress and the Eulerian strain rate. No connection with the classical concept of stability is offered.

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