Brief Reports

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Determination of structural instabilities of atomic lattices by means of a Monte Carlo simulation

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We report studies using a simulation technique based on the Monte Carlo method to detect mechanical instabilities of atomic lattices when subjected to various strain histories. As an example of the technique, the zero-temperature mechanical behavior of an initially perfect two-dimensional Lennard-Jones lattice, while subjected to a varying axial strain, is investigated. Requiring only that the interatomic potential be specified, this technique has the advantage over previous schemes in that it does not rely on assumptions concerning the type of deformation imposed upon the lattice.

I. INTRODUCTION

The detection of mechanical instabilities of an atomic lattice offers the ability to predict the ultimate strength of a perfect crystal and to study dislocation and crack nucleation resulting from various strain histories. To date, this approach has been used primarily for the determination of ideal or ultimate strength of various types of crystal-lattice models when subjected to mechanical strain.[1-3] Comprehensive reviews of this work have been given by both Kelly[4] and Macmillan.[5] These investigations depend upon a stability criterion to identify the state of ideal strength of the model. This approach was first proposed by Zwicky[6] using a criterion that was later modified and improved upon by Born and Fürth.[7,8] It states that the ideal strength is reached whenever the lattice, while subjected to an axial strain, becomes unstable against an additional small arbitrary deformation. However, in practice, this criterion to detect lattice instability is approximated by imposing only small *homogeneous* deformations. Kelly[4] has shown that this restriction to homogeneous deformations does not ensure stability against perturbations in strain of a more general nature. In addition to the detection of ultimate strength, a similar criterion can be applied as well to the detection of the onsets of dislocation and crack nucleation, as will be discussed further in the present work.

It is the intent of this paper to describe a simulation technique and to demonstrate its usefulness in detecting the instabilities of a simple model consisting of a two-dimensional Lennard-Jones lattice, subjected to varying axial strain. In Sec. II the methodology of the simulation technique is outlined in detail. Section III contains a description of the example model used in this study with its behavior in response to a specific strain history reported in Sec. IV. The paper concludes with Sec. V, which contains a discussion of the simulation technique and its application to more realistic models.

II. METHODOLOGY OF SIMULATION TECHNIQUE

Here, our objective is to detect structural instabilities of a model system subjected to various loading histories. The simulation technique is based on the Monte Carlo method, which consists of generating a representative group of states from the canonical ensemble of a system at a given temperature. This is accomplished by generating a new atomic configuration from the current one by randomly moving one particle. If the potential energy of the system is reduced by the move, the new configuration is accepted. If the potential energy increases, the configuration is accepted according to the Boltzmann factor $\exp(-\Delta E/kT)$, where ΔE is the difference in potential energy associated with the move. This procedure is iterated until an acceptable approach to equilibrium is achieved. This method has been extended by the present authors[9] to model systems which experience time varying external constraints at a rate of change which is either slow or fast with respect to the rate associated with a lattice equilibration time. In the present study the technique is used to simulate lattice response to the application of axial strain at a rate small enough, such that the lattice remains in a state of local equilibrium. The dynamical loading of the lattice is represented by a finite concatenation of states, each of which is subjected to a set of static external constraints which are differentially varied from one state to the next.

For the case of axial strain, at each state the lattice is initially subjected to a homogeneous deformation that rescales the vertical coordinates of the atomic positions (either compressively or expansively) by one part in 10^5 while holding the horizontal coordinates fixed. The new lattice configuration is then relaxed towards local equilibrium using the Monte Carlo method outlined above.

This relaxation of the atomic positions results in a microscopic deformation field that is no longer necessarily homogeneous. To ensure local equilibrium, the rescaling of atomic positions proceeds for 50 Monte Carlo steps per particle (MCS/particle) after which the lattice is then relaxed for 100 MCS/particle so that the structure remains near a state of local equilibrium. This prescription is repeated as long as the lattice strain energy varies smoothly. Abrupt transitions in the energy, reflecting the lattice instabilities, are treated separately by first locating the strain at which they occur and then applying the Monte Carlo method to equilibrate the lattice at that strain. The complete procedure outlined above has been implemented on a CRAY-1S computer.

As previously mentioned, the interest here is to detect mechanical instabilities while subjecting the lattice model to mechanical strain of a specific nature. The resulting lattice states, however, may be metastable and appear stable only when the thermal energy of any state is far less than the depth of the metastable energy well. In view of this, the investigation of mechanical behavior of the model described in Sec. III is simplified by assuming the condition of zero temperature.

III. MODEL

The simple model, used here for illustrative purposes, is based upon a two-dimensional atomic lattice composed of 360 argon particles, which interact by means of a pairwise Lennard-Jones (LJ) potential, truncated at a radius of 10 Å. The form of the interatomic potential is

$$\phi(r)=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right], \tag{1}$$

where for argon, ε and σ assume the values of 1.877×10^{-14} ergs and 3.368 Å, respectively.[8] As determined in an earlier work,[9] the initial configuration of the lattice is that of a triangular or two-dimensional hexagonal close-packed (hcp) system [see Fig. 1(a)][10] which is in equilibrium at zero temperature and pressure with a nearest-neighbor separation of 3.747 Å.

The model system used in the present work consists of the hcp lattice as described above configured into 18 rows by 20 columns of atoms. The lattice is constrained to obey periodic boundary conditions on its top and bottom boundaries and free-surface conditions on its lateral boundaries. Thus the lattice is topologically mapped onto a cylinder where the application of axial strain is equivalent to changing the radius of the cylinder while allowing its length to vary in response to that change.

IV. RESULTS

As an illustrative example, we have simulated the dynamic response of the lattice model described in Sec. III to a strain history consisting of monotonically increasing axial compressive strain from 0 to 20% (see Fig. 2), and the release of strain from various initial points along the loading curve (see Fig. 3). As shown in Fig. 2, the lattice energy increases monotonically with the application of axial compression prior to 14.3% strain. In this region the lattice structure is simply the initial hcp structure homogeneously compressed in the direction of applied strain and extended homogeneously in the transverse direction as graphically depicted in Fig. 1(b). The model system thus exhibits a Poisson effect. However, above roughly 5% strain, the perfect structure of the lattice is modified with the appearance of small perturbations in the atomic positions. These perturbations, illustrated in exaggeration in Fig. 1(c), represent the departure of the atoms from a homogeneously deformed lattice structure, where lines of atoms diagonal to the direction of applied strain transform into very slight zigzag patterns about the diagonal. Typical displacements of these perturbations with respect to the homogeneously deformed perfect structure are on the order of 10^{-2} Å, and become more pronounced as the compressive strain is increased. At 14.3% axial compression, a lattice instability is encountered, possibly induced by uncontrolled growth of these perturbations in the deformation field. As seen in Fig. 2, the scaled strain energy $[E(0)-E(\epsilon)]/E(0)$ decreases abruptly from 51 to 4% with the ensuing state, depicted in Fig. 1(d), displaying a mildly distorted hcp lattice with the inclusion of a few dislocations. Thus this transition is associated with the lattice displaying its ultimate strength and the energy necessary to nucleate lattice defects from an initially perfect structure. Subsequent to this transition, the lattice is then compressed to a maximum axial strain of 20%. At approximately 16% compression, the dislocations coalesce to form a slip line through the lattice oriented at roughly 45° to the direction of applied strain. Beyond this point, the lattice responds to the additional axial compression with a display of slippage of lattice sections at their common boundary defined by the slip line. This response results in a translation of the lattice sections in the direction perpendicular to that of applied strain, thereby increasing the total transverse lattice dimension.

Lattice response has also been calculated for the

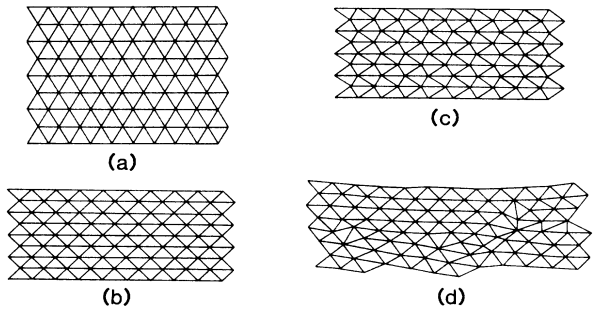

FIG. 1. Schematic lattice configurations of an internal section of the lattice at various axial strains (Ref. 10). (a) A section of the initial unstrained two-dimensional hcp lattice, wherein the atoms are located at the vertices of a nested collection of equilateral triangles. (b) Lattice configuration for compressive strains less than 5%. The lattice is homogeneously compressed in the direction of applied strain and extended in the transverse direction thereby exhibiting a Poisson effect. (c) Lattice structure at strains between 5% and 14.3% in absence of any strain energy release. Here, the lattice displays small zigzag perturbations in the atomic positions. (d) Lattice structure at strains greater than 14.3%. The lattice exhibits a mildly distorted hcp structure along with the inclusion of dislocations.

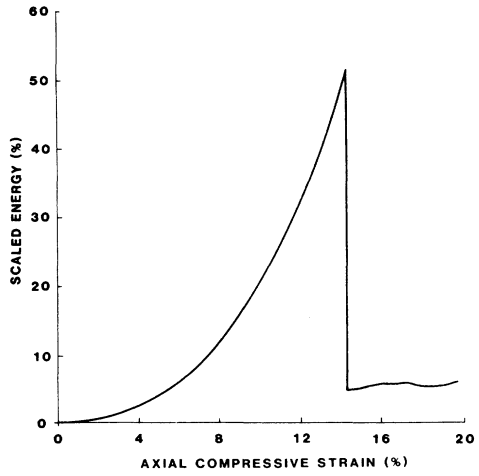

FIG. 2. Scaled energy $[E(0)-E(\epsilon)]/E(0)$ vs axial compressive strain ϵ for the loading curve out to 20% strain. $E(0)$ is the initial lattice energy at 0% strain with $E(\epsilon)$ representing the lattice energy corresponding to the strain ϵ.

release of compressive axial strain to zero starting at various points along the loading curve in Fig. 2 prior to the transition at 14.3% strain. Only those release paths starting from the maximum compressive states at 5%, 9%, and 12% axial strain are displayed in Fig. 3. The nature of all the release paths calculated suggest the existence of three regimes of mechanical response for this particular model prior to the transition from perfect to defective structure. The first regime, labeled I, extends from 0% to approximately 5% maximum compressive strain and reflects a purely elastic mechanical response. A release path initiated from any state within this regime will overlay the loading curve. In addition, all of the compressive strain energy is recovered upon release, with no residual lattice damage suffered.

The second regime (II) is defined by the set of maximum compressive strains lying approximately between 5% and 10%. At the compressive states in this regime,

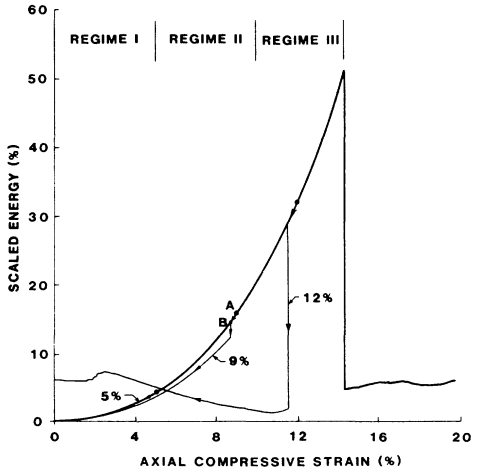

FIG. 3. Scaled energy $[E(0)-E(\epsilon)]/E(0)$ vs axial compressive strain ϵ showing the release curves from 5%, 9%, and 12% maximum compressive strain.

the lattice exhibits a locally elastic response where the unloading curve initially follows the loading path for roughly 0.3% release of strain (e.g., points A to B in Fig. 3). Upon further release, the lattice structure becomes unstable and experiences a transition, which, as illustrated in Fig. 3 by the release curve from 9% axial compression, relieves about 15% of the strain energy. The physical change in the lattice associated with the transition is nothing more than an intensification of the zigzag perturbations in the atomic positions from their otherwise homogeneously strained hcp locations. This results in roughly a 1% increase in the overall lattice dimension perpendicular to the direction of applied strain, thereby causing a decrease in the lattice strain energy. As the unloading process continues, the zero-stress state is found to occur at 0% compression where full recovery of the lattice strain energy has occurred.[11] Thus the compression-release cycles possessing maximum strains within this regime illustrate an anelastic behavior of the lattice. That is, the release path is not coincident with the load curve (indicative of inelastic behavior), whereas the lattice strain energy is fully recovered with no permanent lattice damage.

The third regime (III) of lattice model behavior lies between the second regime and the 14.3% transition, and thus involves those values of maximum compressive strain between 10% and 14.3%. Here, as in regime II, the lattice exhibits a locally elastic response when subjected to a maximum compressive strain lying within this regime. However, the instability and subsequent transition which occur as unloading proceeds, results in a lattice state that is qualitatively similar to that resulting from the 14.3% transition, i.e., a hcp lattice exhibiting dislocations. In the case of release from a maximum axial compression of 12% (see Fig. 3), the onset of instability occurs at 11.5% strain, resulting in a substantial reduction of the lattice strain energy. As unloading continues beyond the transition, the lattice quickly experiences a zero-stress state (located at the energy minimum in the release path) at a nonzero value of compressive strain, thereby indicating the presence of permanent deformation. In particular, for the 12% unloading case, the zero-stress state occurs at a compressive strain of 10.7% relative to the original uncompressed lattice. The appearance of the permanent deformation implies that the lattice structure has sustained damage, where the difference in lattice energies corresponding to the initial and zero-stress states represents a quantitative measure of this damage. As the lattice is placed in tension beyond the zero-stress state, it experiences an axial tensile strain which eventually leads to crack nucleation and growth initiated at the sites of existing lattice defects. For the release path displayed in Fig. 3 starting from 12% maximum compression, the strength of the lattice is undermined by crack nucleation and growth, as indicated on the release path at the somewhat noisy transition at roughly 2.3% compressive strain relative to the original uncompressed lattice or 8.4% tensile strain relative to the zero-stress state. It is emphasized here that these results have proved to be independent of the aspect ratio of the lattice and the number of particles compris-

ing it. In addition, the results have displayed no sensitivity to a large increase in the number of Monte Carlo steps used in the simulation technique, which would otherwise suggest metastability.

V. DISCUSSION

Despite the simplistic nature of the model considered here, it exhibited an unexpected and unusual mechanical response. Whether similar behavior is displayed by more realistic models remains to be seen; however, the point we wish to emphasize here is the ability of the simulation technique to detect the various instabilities displayed by the model. As stated earlier, previous investigations into the response of atomistic models of solids have concentrated primarily on the determination of ultimate strength. These approaches were loosely based on the criterion that the ultimate strength is reached whenever the lattice, while subjected to an axial strain, becomes unstable against an additional small, homogeneous deformation. As mentioned previously, the restriction to homogeneous deformations does not, in general, rule out lattice instability against arbitrary deformations. In addition, there exist only a few attempts[1,7] to study the stability of the deformed crystal lattice, whereas most investigations have tacitly assumed that the lattice remains stable at all strains. However, the simulation technique reported here is not subject to these limitations. By incorporating the Monte Carlo method into the technique, we avoid the restriction to homogeneous deformations by introducing small arbitrary deformations in a manner which naturally leads to a state of local lattice equilibrium. In addition, as shown by the results reported in Sec. IV, this technique cannot only detect the instability associated with the ultimate strength of the lattice model, but also those associated with the onset dislocation and crack nucleation during the imposition of complex strain histories.

The inadequacies of the stability criterion, as based on homogeneous deformations alone, is illustrated through its inability to detect several features of lattice behavior displayed by the present model. First, as displayed in regimes II and III of Fig. 3, the existence of locally elastic behavior in the neighborhood of a maximum compressive state implies that the instability encountered during release of axial strain cannot be detected by a perturbation stability analysis. Second, the zigzag perturbations in the deformation field, which lead to the instability of the lattice, do not constitute a homogeneous deformation. Thus the physical consequences of such perturbations would remain undetected by previous investigations. Third, the nature of the dynamical simulation introduced by the present authors provides for the detection of instability of the deformed lattice in any state along a complex strain history, by allowing initially small perturbations to evolve in response to the variation in the external constraints imposed upon the lattice. Indeed, the fundamental mechanism leading to the unusual mechanical response displayed by the model in regimes II and III is the growth of initially small, inhomogeneous perturbations in the deformation field. The reason that the lattice behaves anelastically in regime II as opposed to the inelastic behavior displayed in regime III is simply that the lattice possesses an insufficient amount of strain energy to nucleate dislocations.

Whether this unusual behavior persists at nonzero temperatures remains to be determined. However, the finite neighborhoods associated with the locally elastic behavior exhibited by the lattice suggests that this behavior will persist at nonzero, although possibly small, temperatures. At higher temperatures, it is possible that the thermal energy-induced perturbations to the lattice strain energy will cause the locally elastic behavior, displayed in regimes II and III, to disappear. If so, it seems reasonable to expect the mechanical behavior at such temperatures to be partitioned into the more conventional regimes of elastic and inelastic response.

In summary, we have introduced a new technique involving the Monte Carlo method to simulate the mechanical response of atomic lattices to an imposed complex strain history. This technique is particularly sensitive to detection of the onset of structural instabilities. It is aptly suited to implement the criterion of Born and Fürth in detecting the instabilities associated with the ultimate strength and nucleation of lattice damage. This technique is applicable to more general lattice models than that considered here, and requires only the specification of an interatomic potential function to model interactions between the various atoms or molecules of the system.

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[10]Figure 1 is a schematic representation of an internal section of the lattice only and therefore does not necessarily reflect the periodic boundary conditions imposed on the top and bottom boundaries of the lattice.

[11]Due to the nature of the Monte Carlo technique used here, the dynamical simulation is isothermal in nature. Thus the residual thermal energy associated with the hysteresis of the compression-release cycles is not accounted for in the calculations.