ISSN 1028-3358, Doklady Physics, 2014, Vol. 59, No. 8, pp. 372–374. © Pleiades Publishing, Ltd., 2014.
Published in Russian in Doklady Akademii Nauk, 2014, Vol. 457, No. 5, pp. 539–541.

MECHANICS

Equilibrium and Stability of HCP Crystal Structures under Finite Strain[1]

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Presented by Academician N.F. Morozov February 17, 2014

Received February 25, 2014

DOI: 10.1134/S1028335814080060

In order to ensure the operability of the material and to predict the limit states, it is necessary to introduce models of fracture at different scale, which take into account the internal structure of the material [1, 2]. Herewith, both from scientific and practical points of view, it is particularly important to study the behavior of materials with perfect geometric structure, due to the fact that crystal structure is typical for metals, which are widely used as structural materials. Furthermore, in connection with the advance in nanotechnology single crystals are becoming more and more demanded, and their strength is close to theoretical, or ideal. One of the possible causes of fracture is the loss of stability of the material's internal structure, thus in the experimental measurement of the ideal strength it is necessary to check the stability with respect to any additional small distortion at each stress or strain increment [2].

In this paper discrete-continuum approach is applied to stability investigation of crystal structures. Long-wave approximation is used for homogenization, and then continuum analysis is carried out. Cauchy–Born rule [3] is employed to relate macroscopic deformation of crystals with the changes in lattice vectors. If the lattice is simple, i.e., coincides with its Bravais lattice, the change in the position of each particle is described by the same strain gradient as the macroscopic deformation. Further stability investigation for simple lattices is done, e.g., in [7, 8]. For multi-lattices this rule is to be modified because of the internal degrees of freedom. One of the variants, which is used in the present work, is introduced in [5]. The review on modifications of Cauchy–Born rule is done in [6].

In order to describe the material in the reference configuration, let us introduce a coordinate system and draw particles radius-vectors. Following [4], let an arbitrary particle have number 0, others will then have numbers $k = 1, 2, ..., N$. HCP structure is characterized by diatomic lattice, for which the relation between bond lengths and directions has the form [5]:

$$a_k \mathbf{e}_k = a_k^0 \mathbf{e}_k^0 \cdot \overset{\circ}{\nabla} \mathbf{r} + \nu_k \boldsymbol{\xi}, \tag{1}$$

where a_k and $\mathbf{e}_k$ are bond length and direction in current configuration, a_k^0 and $\mathbf{e}_k^0$ are bond length and direction in reference configuration, $\mathbf{r}\overset{\circ}{\nabla} = (\overset{\circ}{\nabla}\mathbf{r})^T$ is strain gradient [9], $\nu_k = 0$, if zero and kth particles belong to one sublattice, $\nu_k = 1$, if zero and kth particles belong to different sublattices, $\boldsymbol{\xi}$ is sublattice shift vector.

In this work let us confine ourselves to pair force interaction hypothesis. Strain energy (Cauchy–Born energy) for this material model is [4, 10]:

$$W = \frac{1}{2V_0}\sum_k \Pi_k, \quad \Pi_k = \Pi(a_k), \tag{2}$$

where V_0 is unit cell volume in reference configuration, $\Pi = \Pi(r)$ is pair force potential, which depends only on the distance between particles.

Equilibrium equations in reference configuration for the equivalent continuum have the form:

$$\begin{gathered}\frac{\partial W}{\partial(\overset{\circ}{\nabla}\mathbf{r})} = 0 \Rightarrow \sum_k \Pi'\left(a_k^0\right) a_k^0 \mathbf{e}_k^0 \mathbf{e}_k^0 = 0, \\ \frac{\partial W}{\partial \boldsymbol{\xi}} = 0 \Rightarrow \sum_k \nu_k \Pi'\left(a_k^0\right) \mathbf{e}_k^0 = 0.\end{gathered} \tag{3}$$

Normally the second equation holds identically, and the first one is used to determine so-called com-

[1] The article was translated by the author.

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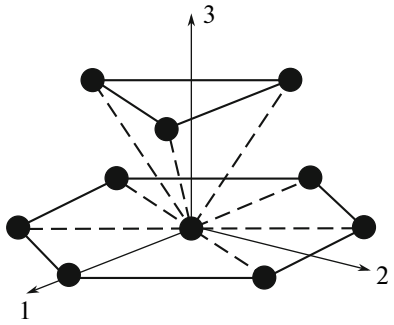

Fig. 1. Typical parts of HCP and FCC structures and eigenvectors of strain gradient.

pression of bonds [4]: when more than one coordination sphere is taken into account, equilibrium distance between nearest neighbors is smaller than the equilibrium distance of the potential.

After a uniform strain is imposed, the second equation determines the shift of the sublattices:

$$\frac{\partial W}{\partial \xi} = 0 \Rightarrow \sum_k \nu_k \Pi_k' \mathbf{e}_k = 0, \quad \Pi_k' = \Pi'(a_k). \qquad (4)$$

As the deformation of the sublattices themselves is homogeneous, no additional equilibrium condition is required.

Further, energy stability criterion (5) is used, i.e. second variation of strain energy is required to be positive [11]. It can be shown that for simple lattices it is equivalent to the condition of strong ellipticity of the equilibrium equations, which is necessary condition for uniformly deformed material [9]. In addition, for simple lattices strong ellipticity condition is also sufficient in current assumptions [7, 8].

$$\delta^2 W > 0 \Leftrightarrow \begin{cases} \delta(\mathbf{r}\mathring{\nabla}) \cdot\cdot\, {}^4\mathbf{Q}_* \cdot\cdot\, \delta(\mathbf{r}\mathring{\nabla}) > 0, \\ \delta\xi_* \cdot {}^2\mathbf{Q} \cdot \delta\xi_* > 0, \end{cases} \qquad (5)$$

$$\forall \delta\xi_*, \quad \forall \delta(\mathbf{r}\mathring{\nabla}),$$

where

$${}^4\mathbf{Q}_* = {}^4\mathbf{Q} - {}^3\mathbf{Q}^T \cdot {}^2\mathbf{Q}^{-1} \cdot {}^3\mathbf{Q},$$

$$\delta\xi_* = \delta\xi - {}^2\mathbf{Q}^{-1} \cdot {}^3\mathbf{Q} \cdot\cdot\, \delta(\mathbf{r}\mathring{\nabla}),$$

$${}^4\mathbf{Q} = \frac{\partial^2 W}{\partial(\nabla\mathring{\mathbf{r}})^2} = \frac{1}{2V_0}\sum_k \left[\frac{1}{a_k^2}\left(\Pi_k'' - \frac{\Pi_k'}{a_k}\right)\mathbf{a}_k^0\mathbf{a}_k\mathbf{a}_k^0\mathbf{a}_k + \sum_n \frac{\Pi_k'}{a_k}\mathbf{a}_k^0\mathbf{i}_n\mathbf{a}_k^0\mathbf{i}_n \right], \qquad (6)$$

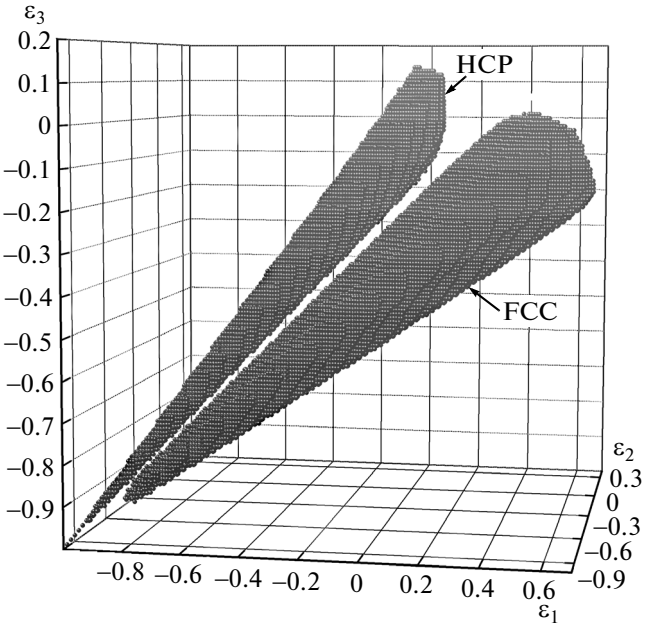

Fig. 2. HCP structure stability regions, Lennard-Jones potential. Left region corresponds to stress-free HCP structure, right region corresponds to stress-free FCC structure.

$${}^3\mathbf{Q} = \frac{\partial}{\partial\xi}\left(\frac{\partial W}{\partial(\mathring{\nabla}\mathbf{r})}\right)$$

$$= \frac{1}{2V_0}\sum_k \left[\nu_k\left(\Pi_k'' - \frac{\Pi_k'}{a_k}\right)\mathbf{a}_k^0\mathbf{e}_k\mathbf{e}_k + \nu_k\frac{\Pi_k'}{a_k}\mathbf{a}_k^0\mathbf{E} \right],$$

$${}^2\mathbf{Q} = \frac{\partial^2 W}{\partial\xi^2} = \frac{1}{2V_0}\sum_k \left[\nu_k\Pi_k''\mathbf{e}_k\mathbf{e}_k + \nu_k\frac{\Pi_k'}{a_k}(\mathbf{E} - \mathbf{e}_k\mathbf{e}_k) \right].$$

Here, $\mathbf{E} = \sum_n \mathbf{i}_n\mathbf{i}_n$ is unit tensor, $\mathbf{i}_n$ are basis vectors, $n = 1, 2, 3$ is space dimension.

Shift vector ξ components, which enter the condition (5), are determined from (4) for each current configuration. For the HCP structure's symmetry reasons, if one of the strain gradient $\mathbf{r}\mathring{\nabla}$ eigenvectors coincides with the axis of transverse isotropy, and the other two lie in the plane of isotropy, then ξ also lies in the plane of isotropy.

Let us further restrict ourselves to such $\mathbf{r}\mathring{\nabla}$, whose eigenvectors are shown in Fig. 1. Lennard-Jones potential is used as an example of pair force interaction potential:

$$\Pi_{LJ}(r) = D\left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^6\right], \qquad (7)$$

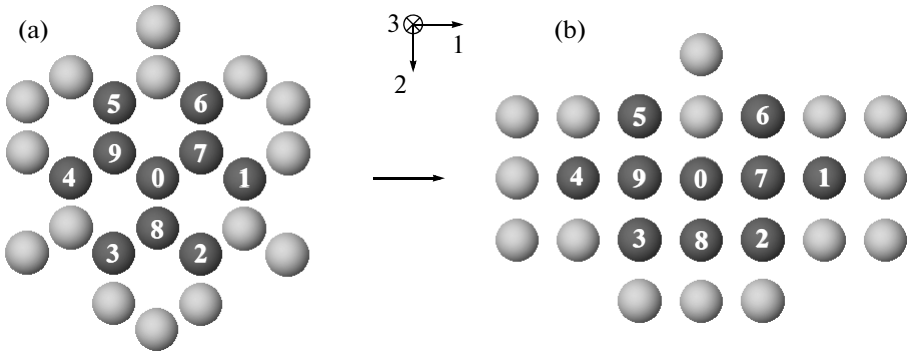

Fig. 3. Example of HCP (a)–FCC (b) transition.

where D is the depth of the potential well, a is equilibrium distance.

Figure 2 shows the stability region of HCP structure, ε_1 and ε_2 describe the deformation in the plane of isotropy, ε_3 describe the deformation along the axis of transverse isotropy. ($1 + \varepsilon_1$, $1 + \varepsilon_2$, $1 + \varepsilon_3$ are the principal values of the strain gradient). Stability region consists of two domains containing two stress-free states: the first one with coordinates $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 0$ corresponds to HCP structure, the second one with coordinates

$$\varepsilon_1 = \sqrt{2} - 1, \quad \varepsilon_2 = \sqrt{\frac{2}{3}} - 1, \quad \varepsilon_3 = \frac{\sqrt{3}}{2} - 1$$

and sublattice shift vector

$$\xi_1 = 0, \quad \xi_2 = a\frac{\sqrt{2}}{6}, \quad \xi_3 = 0,$$

which ensures equilibrium (4), corresponds to FCC structure. Analogously to the triangular lattice [7], the presence of two stability domains does not depend on the specific form of the interaction potential (Lennard-Jones, Morse, Mie).

Continuous straining path from cubic to hexagonal lattice was first described in [12]. Subsequently, another transitions were proposed, e.g., [13]. The technique, which is used in the present work, allows us to study all possible straining paths which connect two stress-free states. Figure 3 shows stress-free HCP and FCC structures from Fig. 2, projected onto the plane 1–2. Grey color marks zero particle and its twelve closest neighbors in HCP structure.

The obtained stability conditions are valid in the space of any dimension for any diatomic lattice within pair force interaction, and they can be extended to the cases of multi-lattices and more sophisticated interaction laws. The present technique allows to obtain stability region in strain space for the material with microstructure. The possibility to describe various straining paths, which connect stress-free states, is illustrated by the analysis of two stability domains containing stress-free HCP and FCC structures.

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