UDC 539.4

Effects of Lattice Relaxation and Limiting Shear Stress of fcc Metals at High-Rate Deformation

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УДК 539.4

Влияние релаксации решетки и предельного напряжения сдвига ГЦК-металлов при высокоскоростном деформировании

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Представлены результаты расчетов теоретического предела сдвига для ГЦК-металлов Cu, Ni, Ag, Au, Pd, Pt с применением "универсальных" эмпирических потенциалов межатомного взаимодействия типа погруженного атома. Показано, что эффекты релаксации решетки играют важную роль в формировании промежуточних дефектных структур и приводят к значительному уменьшению соответствующих значений теоретического предела текучести. Обсуждаются эффекты "антиадиабатического" влияния на предельную прочность материала в условиях высокоскоростного нагружения.

Introduction. The existence of the limiting shear stress plays an important role in the processes of formation and propagation of shock waves in solids. Therefore, for each quantitative theory of impact, it is necessary to take into account impingement or other high-rate deformation processes, where a solid material is present. An important feature of the limiting shear stress in the process of high-rate deformation is its dependence on the strain rate. Under conditions of impact, this dependence may be quite strong (note, for example, that in [1] the concept of "the ultimate velocity of deformation" has been proposed), but its physical nature is not yet clear. To address this problem, we consider the simplest model for $\tau_{\max}$ similar to the classical Frenkel model [2]. The difference is that we take specific crystallographic structure (fcc structure), use true model of interatomic interactions ("universal" embedded atom potentials [3, 4] from [5]), and allow for full atomic relaxation during the shear process. The purpose is to investigate quantitatively the influence of the effects of lattice relaxation on the magnitude of $\tau_{\max}$. With the assumption that $\tau_{\max}$ is limited by its "theoretical limit" (in the sense that neither cracks nor plastic deformation are present), one can distinguish the "low-rate" and "high-rate" regions by the ability of atoms to follow the most preferable (energetically) path of the deformation process. In the limiting cases of infinitely slow and infinitely fast deformation, this corresponds to the "adiabatic" (for a given macroscopic deformation, the atomic configuration corresponds to the global minimum of potential energy) and "anti-adiabatic" (atomic positions are fixed by external conditions and no local relaxation is allowed) limits. The actual relation $\tau(\dot{\varepsilon})$ must lie somewhere between those limits.

Results of Modeling. Six materials with fcc lattices were investigated. Two shear planes were considered with two directions of shear in each plane: [100] and [110] for the (001) plane, and $[1\bar{1}0]$ and $[\bar{2}11]$ for the (111) plane.

In Fig. 1, the energies of non-relaxed sheared configurations are presented. In order to omit obvious dependence of U on the lattice parameter and shear modulus G, the units $G \cdot b$ and b were used for U and x, respectively; b is the atomic lattice parameter in the shear direction.

As it could be expected, the peaks of the curves in Fig. 1 are in agreement with Frenkel's estimation (according to the latter, the maximum of the curves in Fig. 1 would be at the level of $1/2\pi^2$). The lattice relaxation, if it takes place during the process of deformation, changes significantly the values of the limiting shear stress. This is illustrated in Fig. 2.

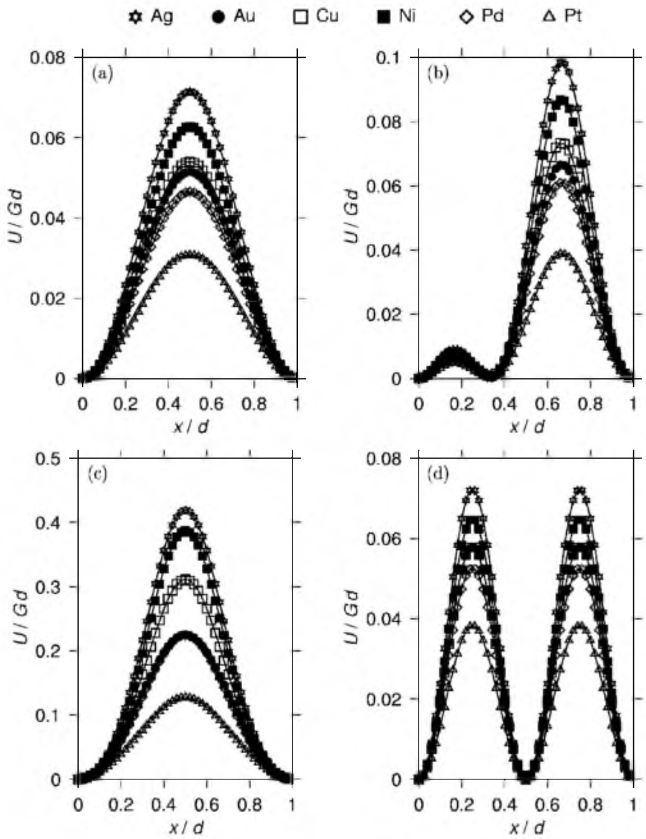

Fig. 1. Dependence of the strain-energy density U on the value of the relative shear x for six fcc metals (no atomic relaxation). Here and in Fig. 2: G is the shear modulus and d is the atomic lattice parameter in shear direction; (a) shear plane (111), shear direction $[1\bar{1}0]$; (b) shear plane (111), shear direction $[\bar{2}11]$; (c) shear plane (001), shear direction [100]; (d) shear plane (001), shear direction [110].

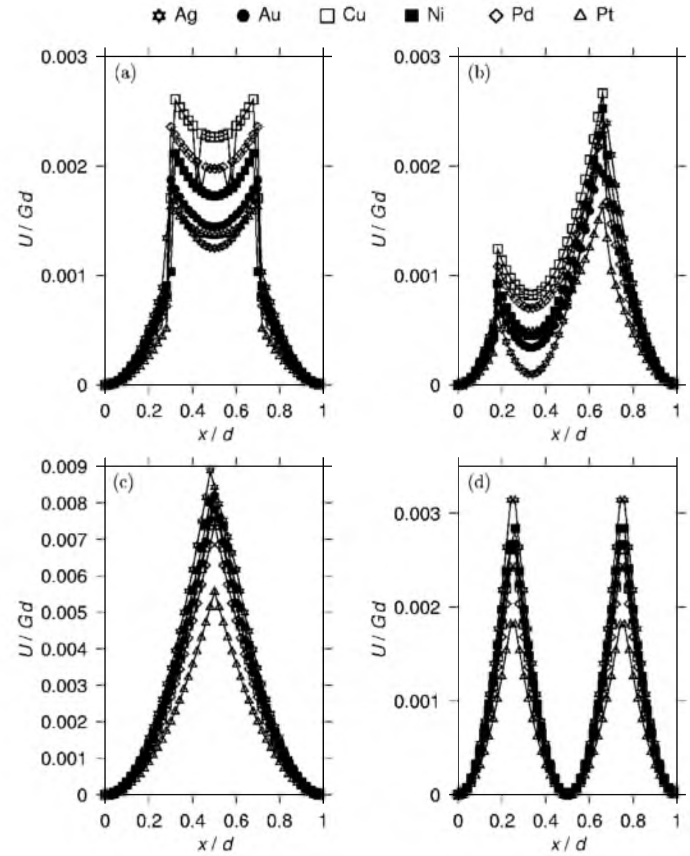

Fig. 2. Dependence of the strain-energy density U on the value of the relative shear x for six fcc metals (full atomic relaxation).

As can be seen from these Figures, the effect of lattice relaxation decreases the "theoretical" value of the limiting shear stress by a factor of 30 and brings it to the order of $10^{-3}G$, which is only 100 times higher than the experimental value typical of metals. This difference can be even smaller. The local minimum between the peaks corresponds to the formation of the stacking fault, and the height of the left minimum corresponds to the minimum energy spent for its formation. If the direction of deformation changes at the point of the minimum energy, one can get resulting deformation in $[1\bar{1}0]$ or $[\bar{1}10]$ directions and, as a combination of the latter, in an arbitrary direction in the (111) plane. The energy needed for such processes is now completely determined by the height of the first peak in Figs. 1b and 2b and is, for the relaxed case, of the order of $10^{-4}G \cdot b$.

Discussion and Conclusions. Let us discuss now possible applications of these results. There are situations where the "ideal" mechanism of inelastic deformation may play an important role. This is the case of high-rate deformation, where the rate of deformation exceeds the velocity of cracks (of course, other defects intrinsically present in a real material such as grain boundaries, dislocations, and point defects are still to be taken into account). It follows from our considerations that the deformation rate is higher than the rate of lattice relaxation and the limiting shear stress generally increases by a factor of 30–50.

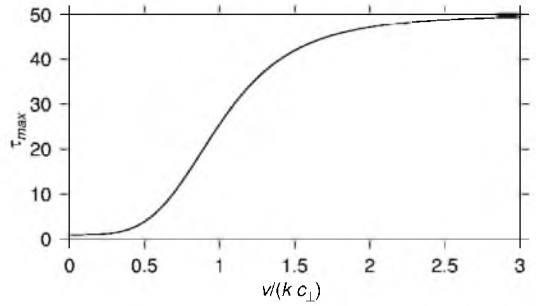

Fig. 3. Possible dependence of the limiting shear stress τ_{max} on the strain rate.

Simple estimations of the lattice-relaxation rate give the value, which is about the speed of sound. Thus, one can expect that the dependence $\tau_{max}(v)$ will be similar to the dependence shown in Fig. 3 (where k is of the order of unity and $c_\perp$ is the speed of sound).

In all probability, the results obtained here for six fcc metals can be directly generalized for other metallic systems due to the similarity of the chemical bonds these materials possess. Systems with covalent bonding need special investigation, and such investigations are now in progress.

Резюме

Наведено результати розрахунків теоретичної границі напруження зсуву для ГЦК-металів Cu, Ni, Ag, Au, Pd, Pt з використанням "універсальних" емпіричних потенціалів міжатомної взаємодії типу зануреного атома. Показано, що ефекти граткової релаксації відіграють важливу роль у формуванні проміжних дефектних структур і приводять до значного зменшення відповідних значень теоретичної границі текучості. Обговорюються ефекти "антиадіабатичного" впливу на граничну міцність матеріалу в умовах високошвидкісного навантаження.

1. V. P. Alekseevskii, "Penetration of a rod into a plate at high velocity," *Fiz. goren. vzryva*, No. 2, 99 – 106 (1966).
2. J. Frenkel, *Z. Fiz.*, **37**, 572–609 (1926).
3. M. S. Daw and M. I. Baskes, "Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals," *Phys. Rev. B*, **29**, No. 12, 6443 – 6453 (1984).
4. M. W. Finnis and J. E. Sinclair, "A simple empirical n-body potential for transition metals," *Phil. Mag. A*, **50**, 45 (1984).
5. S. M. Foiles, M. J. Baskes, and M. S. Daw, "Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys," *Phys. Rev. B*, **33**, No. 12, 7983 – 7991 (1986).

Received 14. 11. 2001