Curvature Solitons as Generalized Structural Wave Carriers of Plastic Deformation and Fracture

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Abstract—A nonlinear wave approach to the description of a deformable solid as a multiscale hierarchically organized system was developed. It is shown that all types of strain-induced defects can be represented as curvature solitons of crystal structure—generalized structural wave carriers of plastic deformation and fracture of solids. The scale of a curvature soliton defines the type of a strain-induced defect. The waves of curvature solitons can be dispersed. A curvature soliton generates a crack if the Gibbs thermodynamic potential in a local curvature zone is positive and the material undergoes structural phase decay.

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1. INTRODUCTION

The theory of plasticity and strength of solids was conventionally developed in the framework of single-scale approaches. Continuum mechanics provides macroscale description of a deformable solid based on Newton’s linear mechanics. Physics of plasticity and strength gives microscale description of strain-induced defects in a translation-invariant crystal. In theories of strain-induced defects, the mathematical apparatus of Newton’s linear mechanics is preserved.

Physical mesomechanics treats a deformable solid as a nonlinear multiscale hierarchically organized system. Particular attention is given to nonlinear behavior of a solid in any external fields. This nonlinearity problem is impossible to solve if we reason from the steady structure of a translation-invariant crystal. Any strain-induced defect is nucleated within a local crystal curvature in the zone of which local structural transformation occurs as a strictly nonlinear process. Therefore, the nonlinearity problem is inevitably related to the mechanisms of local structural transformations in local curvature zones as nonequilibrium thermodynamic processes. It is these issues that we consider in the paper.

2. BASIC NONLINEARITY PHYSICS OF A DEFORMABLE SOLID

The methodology of multiscale description of a nonlinear hierarchically organized system was much contributed by the works [1–3] suggesting that a deformable solid should be considered as consisting of two subsystems: a three-dimensional translation-invariant crystal and a planar subsystem comprising surface layers and all internal interfaces. In the thermodynamically stable translation-invariant crystal, the energy is insufficient for generation of strain-induced defects, whereas the planar subsystem meets all conditions necessary for generation of these defects.

According to the theory [4–7], there are three conditions to be met to provide nucleation and motion of strain-induced defects:

– there should be regions of local tensile normal stresses creating an increased molar volume in which local structural transformation can proceed;

– in these regions, there should operate couple stresses producing local curvature in the zone of which a highly excited nonequilibrium state of material arises;
– in the curvature zone, there should occur new allowed structural states of short-range displacements with their own band of energy states in the electron energy spectrum. If the above conditions are met, highly excited atoms in the local curvature zone transfer from the main lattice nodes to the new allowed structural states forming a strain-induced defect core. This decreases the Gibbs thermodynamic potential in the curvature zone. Hence, any strain-induced defect, being nonequilibrium, is metastable and has its local minimum on the molar volume dependence of the Gibbs thermodynamic potential \( F(v) \) [2, 8].

The first condition (the presence of tensile normal stresses) is associated with a chessboard distribution of tensile and compressive normal stresses at the “planar subsystem–3D crystal” interface [9–11]. Plastic shear at the interface can arise and develop only in the zones of tensile normal stresses. This governs channeling of the plastic flow at the interface and hence on the loading axis, emergence of couple stresses, and formation of curvature in the shear zone.

The formation of crystal structure curvature in the shear zone is a fundamental physical phenomenon in plasticity and strength of solids. The curvature effect develops on several scales, thus providing validity of the second condition for nucleation of strain-induced defects in the planar subsystem. Theoretical description of nano-, micro-, and mesoscale couple stresses in the planar subsystem was given elsewhere [12, 13]. The use of molecular dynamics [14] allowed describing the generation of couple stresses at the interface of two fcc crystals (Cu and Ag) with their chessboard distribution on the nano- and microscales. The linear analytical description with continuum mechanics [15] shows that the normal stresses \( \sigma \) and tangential stresses \( \tau \) at the interface of two different media are given by the relations:

\[
\sigma = \frac{2 \sigma_y}{\sqrt{3}} \sin \frac{x + l_x}{\Delta \sqrt{2}}, \quad \tau = \frac{\sigma_y}{\sqrt{6}} \cos \frac{x + l_x}{\Delta \sqrt{2}},
\]

where \( \sigma_y \) is the yield strength of a near-boundary layer at the interface under uniaxial tension or compression; \( \Delta \) is the thickness of the near-boundary layer involved in plastic deformation; the parameter \( l_x \) is determined by the expression:

\[
l_x = \frac{\sqrt{2}}{2} \left( \frac{\pi}{2} + \frac{n\pi}{\Delta} \right) \Delta.
\]

From the equations for \( \sigma \) and \( \tau \) it follows that the near-boundary layer adjacent to the interface experiences mesoscale compressive and tensile normal stresses periodically alternating along the axis \( x \). The tangential stresses also vary periodically along the axis \( x \) but with a phase shift by \( \pi/2 \). In other words, the tangential stresses have their maximum at the boundaries of mesovolumes which experience tensile normal stresses. In these mesovolumes, they produce curvature necessary for nucleation of strain-induced defects there.

The above phenomena were studied in 3D modeling by the excitonic cellular automata method with regard to the generation of couple stresses at the boundaries of misoriented grains in a loaded polycrystal [16] and the results confirmed the periodic modulation of stress and strain distributions at the grain boundaries. It is this effect that governs plastic strain localization on different structural scales in a deforming solid. It should be emphasized that accounting for couple stresses in the planar subsystem on mesoscales predicts the possibility of rotational mechanisms of plastic deformation. Such wave mechanisms of plastic deformation develop in nanostructured materials [17, 18] and in dynamically loaded coarse-grained materials [19]. More detailed consideration of this issue is given below.

The third condition for nucleation of strain-induced defects and their participation in plastic shear is conceptually most important. The condition implies that new allowed structural states are bound to arise in nonequilibrium curvature zones. This issue was considered in substantiating the concept of highly excited states in crystals [4–6]. The basic criteria for highly excited states are the formation of new structural states in the interstitial space and the change in the number of degrees of freedom of a crystal. As a result, the states are degenerated with respect to various atomic configurations. The motion of elements of the system becomes less deterministic and wave behavior of the ionic subsystem becomes possible. This is bound to result in fluctuation modes in the electron density spectrum of states [4].

The authors of [6] suggest considering the conditions of highly excited states in terms of an ensemble of potential reliefs whose distribution law is specified by a synergetic potential. The rearrangement parameter of the ionic subsystem is determined by correlated variation in a potential relief over macroscopic distances. The collective excitations with critical behavior are reduced to the transverse acoustic phonon branch.

The paper [7] considers the effect of external tension of a 1D crystal on the critical potential energy of a system of pairwise interacting particles. It is shown that if the pair interaction potential of particles has a single minimum, the increase in interparticle spacing results in local minima of the potential of the particle system due to bifurcation.