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PHASE FIELD THEORY OF DISLOCATIONS OBTAINED BY COARSE GRAINING

*** I. Groma[1] and P. Ispánovics[2]**

[1] Eötvös University Budapest,
Department of Materials Physics
H-1518 Budapest POB 32, Hungary
groma@metal.elte.hu,
http://metal.elte.hu

[2] Eötvös University Budapest,
Department of Materials Physics
H-1518 Budapest POB 32, Hungary
ispanovity@metal.elte.hu,
http://metal.elte.hu

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ABSTRACT

In the past decade there has been a increasing activity to develop a continuum theory of dislocations. Theoretical investigations are largely motivated by the experimental finding that if the characteristic size of a specimen is less than about 10μm the plastic response of the crystalline materials depends on the size (size effect). The simplest possible way to account for this effect is to add gradient terms to the ”local” ones in the stress-strain relation. There are several different phenomenological propositions to incorporate gradient terms into continuum plasticity models. Although they are successfully applied to explain certain experimental results, the physical origin of the different gradient terms are not clear.

Since in crystalline materials the elementary carriers of plastic deformation are the dislocations, a continuum theory should be built up from the properties of individual dislocations. For a system of parallel edge dislocations with single slip Groma et al. [1] have established a systematic way to derive a continuum theory from the equation of motion of individual dislocations. The most important feature of this theory is that gradient terms appear naturally in the evolution equations of the different dislocation densities. At the moment, however, it is not clear how to extend the model for more complicated dislocation geometries and configurations. Recently, several new promising frameworks have been proposed for treating curved dislocations with statistical methods, but there are many open issues to be resolved before we can say we have a well established 3D continuum theory of dislocations. Constructing a continuum theory even for 2D multiple slip is far from straightforward.

A dislocation ensemble is a system of objects with long range interaction. So the traditional methods developed for atomic systems to derive a continuum theory from the equation of motion of the individual objects cannot be directly applied. In the investigations presented we consider a set of parallel edge dislocations representing the simplest possible, but already rather complex system.

In the first part of the paper the 3D field theory of individual dislocations developed by Kröner [2] is reformulated into a variational problem [3]. Since the general 3D problem is rather complicated the variational formalism is simplified for the 2D edge dislocation case. It is shown, that if one simple replaces

the different discrete dislocation density fields by their coarse grained counterparts in the energy functional this results in a continuum theory of dislocation that completely neglect dislocation-dislocation correlation effects [4,5]. To account for correlations an energy correction term is proposed. The evolution equations of the different dislocation densities are obtained from this corrected functional by applying the standard formalism of phase field theories.

In order to check if the continuum theory derived is able to account for the collective properties of dislocations its predictions were compared with discrete dislocation dynamics simulations for different static cases. The problem of induced geometrically necessary dislocation density developing around an extra dislocation added to the system (Debye screening) [4,5] is discussed in details.

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