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COMPUTER SIMULATIONS OF DISLOCATION MOTION IN CRYSTALS

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ABSTRACT

Smart materials attract a growing interest. Their very intriguing properties can be observed and explained by the methods and theories developed quite recently. These materials are finding new exciting applications in all branches of technology.

One of the relatively new and relatively unknown effects, which can be applied to generate an interesting class of smart materials, is the magnetoplastic phenomenon in nonmagnetic materials (MPE). MPE has been observed in alkali halides (NaCl, LiF, CsI), in nonmagnetic metals (Zn, Al), and in semiconductors (ZnS, InSb, Si). It was discovered in 1985 at the Institute of Crystallography in Moscow by the group headed by V.I. Alshits [1] and is explained by the well substantiated hypothesis, that the dislocations (line defects of the crystal lattice responsible for the plastic properties of crystals) can be released from the paramagnetic centers under the influence of the applied magnetic field. The effect was confirmed by independent laboratories and the results were published in over one hundred papers (see the references in [2] and [3]).

The reason to using computer simulations to imitate physical experiments, was associated with the possibility of getting additional information which could not be extracted from real measurements, e.g., distributions of lengths of dislocation segments lengths on stationary moving dislocations, and the numbers of the active pinning points on a dislocation when it moves under the magnetic field.

Dislocation moves in a crystal due to the force field exerted on it by other dislocations and/or external loads. The natural obstacles in that motion are point defects (mostly) and other defects of the crystal lattice.

There are several methods used to conduct computer simulations of the dislocation motion in crystals. One of them, known as a rolling circle method (RCM) [4] is shown in Fig. 1(a).

In this approach a new quasistable configuration is established when the circle rotating around the pinning point, at which the depinning act occurres, meets the new point defect and the dislocation jumps to a new position. This method has two important disadvantages: it is impossible to calculate the time used by the dislocation to move from the old configuration to the new one and it is easy to omit some obstacles. In the go back and ahead method (GBAM) (Fig. 1(b)) it is assumed that at the initial moment

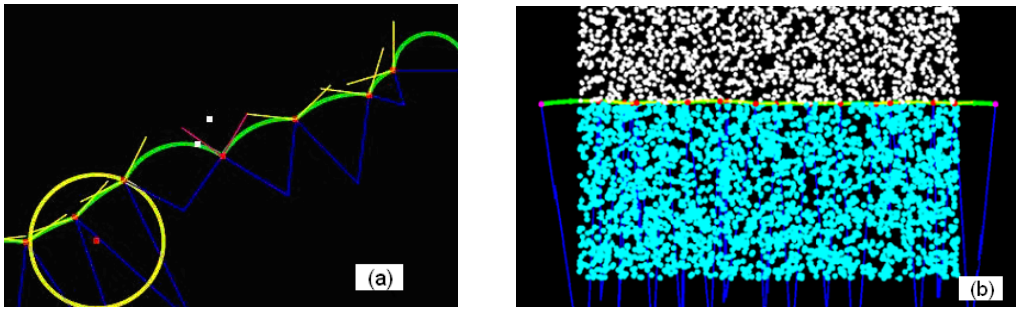

Figure 1: Looking for equilibrium configurations of the dislocation line in the field of point defects; (a) the rolling circle method; (b) go back and ahead method, used by authors

the dislocation is a straight line directed along **L** and situated at the bottom of the observation plane. The point obstacles are supposed to be randomly distributed on this plane. Each of them is characterized by a pinning force f_0. A driving stress $\sigma = \sigma_c$ applied to the dislocation and allowing it to move through the crystal freely without stopping represents a yield point.

During the presentation an algorithm of the GBAM will be explained in details and the results of the computer simulations will be given and discussed.

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