VOLUME 43, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 1979

Edge and Screw Dislocations in an Amorphous Solid

P. Chaudhari and A. Levi
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598

and

P. Steinhardt
Harvard University, Cambridge, Massachusetts 02139

(Received 18 June 1979)

We have studied, using computer simulation techniques, the properties of edge and screw dislocations in an amorphous Lennard-Jones solid. We find the edge dislocation to be unstable and the screw to be stable. The elastic properties of the screw dislocation in the amorphous solid are like those in a crystal.

The existence of edge and screw dislocations in crystals is very well established. Their role in a great variety of solid-state phenomena is known. In contrast, little is known or published about the properties of dislocations in amorphous solids. There has been some discussion recently about their role in the plastic properties of metallic glasses.[1,2] On the other hand, the notion of dislocations as localized line defects in amorphous solids has been questioned.[3] Theories of mechanical properties of metallic glasses, which are currently of great interest, either assume dislocations or deny their existence in developing models for mechanical behavior.[4] Dislocations have been invoked to explain the onset of melting in three-dimensional solids. Computer simulation studies purporting to show "dislocationlike" defects in liquids have been reported.[5] No evidence that these "dislocationlike" defects have the elastic properties of dislocations was presented. It has been suggested by Anderson[6] that the glass transition in amorphous solids may be explained in terms of the Kosterlitz-Thouless theory.[7] Although Anderson appears to speculate that a dangling bond in a random network may be the defect, it appears to us that a starting point may be to examine the viability of the concept of dislocations in amorphous solids and determine if these, as in the other Kosterlitz-Thouless models, play a role. We shall return to this point again at the end of this note.

In this Letter we describe our results of a computer simulation of edge and screw dislocations in an amorphous solid characterized by a Lennard-Jones potential. We find that the edge dislocation is not stable. By this we mean that the elastic properties characteristic of an edge dislocation are not found in an initially dislocated and subsequently relaxed model. We find, however, that the screw dislocation is stable.

The problem of studying dislocations in amorphous solids by computer simulation breaks down into three parts. The first of these is the method of introducing the dislocation. The second is one of ascertaining (preferably visually) that a dislocation has been introduced and what the response of the system has been to the presence of the dislocation. The third part is to quantify the elastic properties of the dislocation. We approached the first by the method of Volterra.[8] The edge dislocation was made both by cutting out a strip of material of width equal to one atom diameter (the Burgers vector) and by shear displacements.[9] The screw dislocation was introduced by suitable displacements.[8,9] The initial displacement vector was equal to an atom diameter. Visual observation was carried out using a reference net. This three-dimensional net mapped out the locations of all atoms in, say, the undislocated model to be used for a screw dislocation. Any subsequent displacement of the atoms was followed by observing the change or distortion of the reference net. This method of observation brings apparent order to the amorphous solid. Quantitative evaluation of the elastic properties of the dislocations was carried out by computing the Airy stress function for the edge dislocation and shear stress for the screw dislocation.

The particular model that we chose for study was generated by Finney.[10] It has approximately 8 000 atoms. For the edge dislocation, we used approximately 4 000 atoms, and for the screw, 5 390 atoms. The range of pair-wise interaction was varied between 1.2 and 2.1 times the atom diameter. All of our relaxations were carried out using the conjugate-gradient technique.[11] In order to verify our procedure and also to provide a reference, we carried out similar calculations on a model of a face-centered cubic crystal relaxed under the same potential.

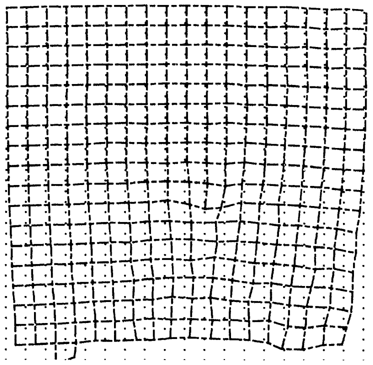

FIG. 1. Reference net of the edge-dislocated amorphous model. The reference model is the cut but unrelaxed starting model. The reference net shows the average motion of atoms on computer relaxation of the reference model.

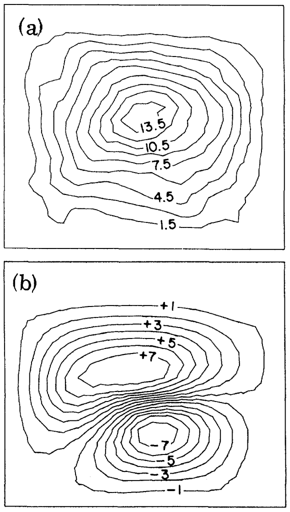

FIG. 2. Airy stress function of the amorphous and crystalline solids in which edge dislocations had been introduced. (a) Amorphous solid; (b) crystalline solid.

The edge dislocation was introduced in a 4193-atom model, roughly $18 \times 18 \times 9$ atoms in dimensions. The dislocation line was parallel to the short direction (the z direction). Prior to introducing dislocation the model is relaxed until its energy-strain curve shows a quadratic behavior. All of the edge-dislocation studies that we describe here were for a pair-wise interaction cutoff distance of 2.1. We have also studied the case where the cutoff distance was 1.2 and found no significant differences in our results. After the model had been relaxed the edge dislocation was introduced in two ways. The top part of the model was displaced relative to the bottom by one or two atom diameters up to the center of the model. This procedure leaves a jog on one side of the model. The model is now relaxed. In the second way of introducing an edge dislocation a cut was made in the model approximately in the lower central half of the model. All of the atoms within this cut, which was equal to an atom diameter, were removed. Before the model was relaxed the remaining atoms were displaced in one of several ways. (1) The atoms were displaced by amounts prescribed by elasticity theory of edge dislocations in a continuum. (2) Atoms in the lower half of the model were moved half an atom diameter inwards towards the cut. (3) Atoms in the lower half were given an inward movement proportional to the distance measured from the center of the cut and parallel to it. (4) No displacement was introduced. In all four cases computer relaxation led to identical configurations and energies. We could not compare the energy between the displaced and cut approaches to generating a dislocation as the number of pairwise interactions involved are different. However, the values of the Airy stress function were very similar leading us to believe that the two methods produce similar final states. Our reason for introducing the edge (and the screw, discussed below) dislocation in different ways was to assure us that our final results were not due to a pecularity of our initial starting conditions and the relaxation process.

With the cut model as a reference model, the reference net readily brings out the relative motion of all atoms in the relaxed model and also the location where the dislocation was introduced. This is shown in Fig. 1. In this net all of the atom motions were averaged over the z direction. We note from the distortion of the net that there is considerable motion of the atoms during relaxation. This motion is locally irregular.

The edge dislocation has four nonzero components of the stress tensor. Rather than compute and plot these separately, it is more convenient to compute the Airy stress function. The different components of the stress tensor can be derived from the Airy stress function. Frank has shown how this can be computed for a model consisting of rods and pinjoints.[12] We have extended and applied his method to compute the Airy stress function for three-dimensional models held together, for example, by Lennard-Jones forces.[13] The Airy stress function of the amorphous model (with an edge dislocation) is shown in Fig. 2(a).

For comparison, the Airy stress function of an edge dislocation in a 4000-atom fcc crystal introduced by the cut-and-weld method described above is shown in Fig. 2(b). The Airy stress function of the dislocation in the crystal has the expected behavior. However, that of the dislocation in the amorphous solid does not. The Airy stress function of the dislocated amorphous solid is very similar to the undislocated and relaxed model, the only difference being in the value of the peak height which is approximately 30% larger in the dislocated and relaxed model.[14] We conclude that an amorphous Lennard-Jones solid has no stable edge dislocation.

For the screw dislocation we used the Finney model again. The model was cut so as to form a cylinder. The diameter of the cylinder was smaller than the width of the original model, and the length was slightly larger than the diameter. Prior to introducing a dislocation, the model was relaxed. The interaction distance was equal to 1.2.

The screw dislocation was introduced in two ways. In the first the z coordinates of all atoms were displaced according to the values given by continuum theory.[9] This displacement results in a screw dislocation along the axis (the z axis) of the cylinder. The model is now relaxed. We show in Figs. 3(a) and 3(b) the reference net of the unrelaxed and relaxed model containing the dislocation. We note that the relaxed model shows some irregular motion of the network, which appears to be confined to the vicinity of the slip plane. We also note that the net is twisted and shows that the relaxation has introduced the Eshelby twist.[9] In the second method of generating the screw dislocation, the displacements along both the z axis and the x-y plane appropriate for a screw dislocation and its accompanying twist were introduced. The model was now relaxed. The resultant screw dislocation could not be distinguished from the first case. Using similar procedures, we introduced a screw dislocation in a 4040-atom crystalline fcc model. The reference net of the crystalline model did not show any irregular motion in the vicinity of the slip plane as had the amorphous model. Other than this difference, the screw dislocation and the accompanying twist were present in both the models. The presence of the twist is indicative of a long-range elastic stress field associated with the dislocation. This was verified by computing the shear stress associated with the dislocation. We show in Fig. 4 the spatial dependence of the shear stress σ_{xz} for the amorphous and crystalline models. The shear stress has the expected spatial dependence.[9] We conclude both from this measurement and the observation of a twist in the reference net that the screw dislocation is a stable defect in amorphous Lennard-Jones solids.

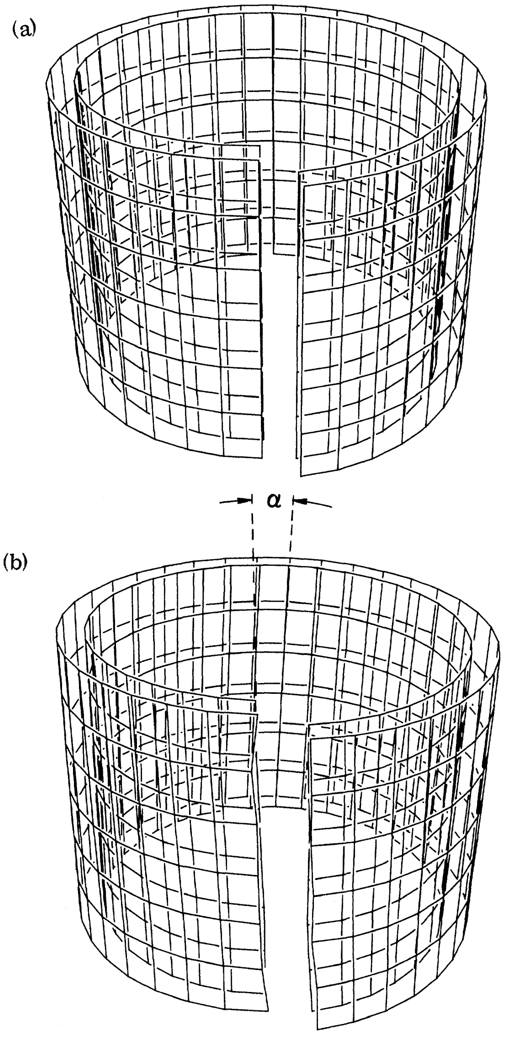

FIG. 3. Reference net of the unrelaxed and relaxed amorphous model containing a screw dislocation. For clarity of presentation, only the two outer segments of the reference net are shown. The presence of the twist in (b) is indicated by the angle.

Our observation that on relaxation an edge dislocation is not stable in an amorphous Lennard-Jones solid is to be compared with our findings on the lack of stability of vacancies in amorphous Lennard-Jones solids.[15] It appears that defects associated with volume changes (dilatational

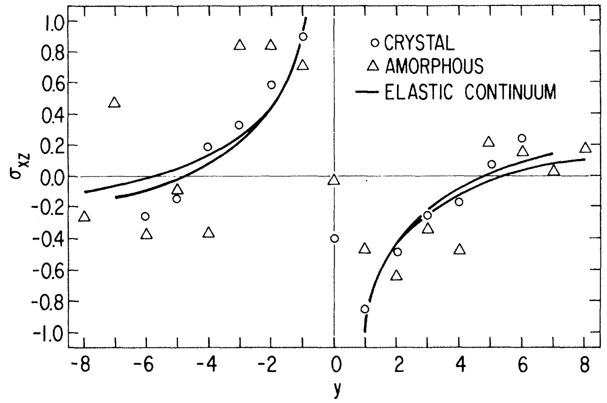

FIG. 4. Calculated spatial dependence of the shear stress of a screw dislocation in a finite cylinder. The two solid curves refer to the two diameters of cylinders. The computed shear stress for the models is averaged over the *z* direction. The shear stress is in arbitrary units, and the *y* axis is in multiples of an atom diameter.

fields) are not stable (metastable). This provides an explanation of annealing and stress-relaxation effects prior to crystallization that are sometimes observed in amorphous solids. The relative lack of kinetic stability of vacancies could also account for the radiation hardness of these materials.

The finding that a screw but not an edge dislocation is possible in an amorphous solid raises many questions. In the absence of edge components, the dislocation line must be straight in a relaxed solid. Dislocation multiplication by sources such as the Frank-Read source is no longer possible. Work-hardening theories, as conventionally applied to crystalline materials, are not applicable. The screw dislocation has one particularly attractive feature from the standpoint of amorphous solids. Its slip plane is not defined as in the case of an edge dislocation; its motion is therefore not restricted to a particular plane. On a speculative level, the presence and motion of screw dislocation could explain the glass-transition temperature. Below this temperature the dislocations are bound and frozen in and can be moved only at high shear stresses. At and above the transition the dislocation pairs unbind and give rise to the glass transition. Above the glass-transition temperature the mobility of the dislocation increases with increasing ability of the structure to adjust its atomic arrangement via increasing amount of free volume[16] with temperature. Our model of the behavior of amorphous solids therefore relies on both the presence of screw dislocations and the free volume.

The authors should like to thank Sir F. C. Frank for suggesting the use of the Airy stress function and for many useful discussions. One of us (P.S.) acknowledges support as a Junior Fellow, Society of Fellows, Harvard University.

---

[1] J. J. Gilman, J. Appl. Phys. 44, 675 (1973).

[2] J. C. M. Li, in *Frontiers in Materials Science*, edited by L. E. Murr and C. Stein (Marcel Dekker, New York, 1976), p. 527.

[3] F. Spaepen, J. Non-Cryst. Solids 31, 207 (1979).

[4] A. S. Argon, Acta Metall. 27, 47 (1979).

[5] R. M. J. Cotterill, Phys. Rev. Lett. 42, 1541 (1979).

[6] P. W. Anderson, in Les Houches Lectures, 1978 (North-Holland, Amsterdam, to be published).

[7] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 5, L124 (1972), and 6, 1181 (1973).

[8] V. Volterra, cited by A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (Dover, New York (1944), p. 221.

[9] J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1968), p. 58; J. D. Eshelby, J. Appl. Phys. 24, 176 (1953).

[10] J. L. Finney, Proc. Roy. Soc. London, Ser. A 319, 479 (1970).

[11] R. Fletcher and M. J. D. Powell, Comput. J. 6, 163 (1963).

[12] F. C. Frank, Phys. Education 13, 258 (1978).

[13] P. Steinhardt and P. Chaudhari, to be published.

[14] The presence of a uniform stress field in the undislocated model is associated with the choice of the cutoff parameter and the pair potential. Reducing the cutoff parameter from 2.1 to 1.2 reduces the peak value of the Airy stress function by a factor of 5. The pair-potential parameters are optimized with respect to an atom diameter. Increasing the cutoff beyond this value results in the observed stresses.

[15] C. H. Bennett, P. Chaudhari, V. Moruzzi, and P P. Steinhardt, to be published.

[16] D. Turnbull and M. H. Cohen, J. Chem. Phys. 52, 3038 (1978).