DISLOCATION MODEL OF POLYSYNTHETIC SHEAR BANDS IN AMORPHOUS MATERIALS

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A dislocation model for a polysynthetic shear band in an amorphous material is proposed. The stress fields near the polysynthetic shear band are calculated. The distribution of impurities in an amorphous binary Fe–B medium containing a polysynthetic shear band is determined.

Key words: amorphous materials, polysynthetic shear bands, calculation model.

The main channel of plastic deformation of amorphous materials is shear bands [1–3]. Normally, they arise in groups and develop in a deformable amorphous material along the direction of the maximum shear stresses. A polysynthetic shear band is understood as a group of parallel shear bands. It is obvious that parallel shear bands are seldom encountered in reality. Usually, they are located at a certain angle to one another. For uniaxial tension or compression, this angle is small. Thus, the concept of polysynthetic shear bands refers to an ideal system which is close to the real system for small disorientation of shear bands.

The theory of polysynthetic shear bands has not so far been developed despite the fact that the shear-band groups are high-stress concentrators and sites of crack nucleation.

The goal of this paper is to calculate the stress field near parallel shear bands using the dislocation model and determine regions of impurity localization near the defects considered.

Figure 1a shows the schematic based on the analysis of the picture of a shear band obtained by high-resolution electron microscopy [1]. One can see from Fig. 1a that the shear band consists of pores and material-adhesion regions located on different sides of the shear plane. According to the dislocation model proposed, the stress fields in the adhesion regions are produced by an edge-dislocation cluster; therefore, the shear bands can be represented in the form of alternating pores and dislocation chains (Fig. 1b).

For simplicity, the length of dislocation chains L and pore size l are assumed to be constant (Fig. 1b). Generally, the values of L and l may differ. We ignore the edge effects associated with the presence of pores in the shear band, which considerably simplifies the expression for the stress fields near the shear bands.

The origin of the Cartesian coordinate system (Fig. 1b) is located at the apex of dislocation clusters. The OX axis is directed along the shear plane and the OY axis is normal to this plane. Knowing the stresses near the unit dislocation [4] and using the superposition principle, one can determine the stress-tensor components for the shear band considered from the relations

$$\sigma_{xx} = -\frac{\mu b}{2\pi(1-\nu)} \sum_{k=0}^{K} \sum_{m=0}^{M} \sum_{n=0}^{N} \frac{y[3(x+nd+m(l+Nd))^{2}+(y+kh)^{2}]}{[(x+nd+m(l+Nd))^{2}+(y+kh)^{2}]^{2}},$$

$$\sigma_{yy} = \frac{\mu b}{2\pi(1-\nu)} \sum_{k=0}^{K} \sum_{m=0}^{M} \sum_{n=0}^{N} \frac{y[(x+nd+m(l+Nd))^{2}-(y+kh)^{2}]}{[(x+nd+m(l+Nd))^{2}+(y+kh)^{2}]^{2}},$$

$$\sigma_{zz} = -\frac{\mu b\nu}{\pi(1-\nu)} \sum_{k=0}^{K} \sum_{m=0}^{M} \sum_{n=0}^{N} \frac{(y+kh)^{2}}{(x+nd+m(l+Nd))^{2}+(y+kh)^{2}},$$
(1)

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Sykhoi Gomel' State Technical University, Gomel' 246746, Belarus. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 44, No. 3, pp. 164–168, May–June, 2003. Original article submitted July 22, 2002; revision submitted October 23, 2002.



Fig. 1. Schematic (a) and dislocation model (b) of a shear band: 1) material-adhesion regions located on different sides of the shear plane; 2) pores; 3) shear plane.

$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\nu)} \sum_{k=0}^{K} \sum_{m=0}^{M} \sum_{n=0}^{N} \frac{(x+nd+m(l+Nd))[(x+nd+m(l+Nd))^2 - (y+kh)^2]}{[(x+nd+m(l+Nd))^2 + (y+kh)^2]^2},$$

where μ is the shear modulus, b is the Burgers vector, ν is Poisson's ratio, $M = L_{SB}/(L+l)$ is the number of pores, L_{SB} is the length of the shear band, N = L/d is the number of dislocations in the cluster, d is the distance between dislocations in the cluster, K is the number of shear bands that form the polysynthetic shear band, and k, m, and n are the summation indices.

Figure 2 shows the parameters of polysynthetic shear bands. It is assumed that the length of all shear bands is identical and equal to L_{SB} and the distance between the bands is also identical and equal to h.

Note, for K = 0, formula (1) yields the stress fields near the unit shear band.

Figure 3 shows the calculation results. The filled and open points refer to the regions of minimum and maximum stresses, respectively. In the region considered, the stresses σ_{xx} are negative and localized in the materialadhesion regions located on different sides of the shear band (Fig. 3a). In this case, these regions are located above one another (see Fig. 2).

Symmetric arrangement of dislocation clusters affects the distribution of other stresses. The stresses σ_{yy} are sign-variable (see Fig. 3c). It is worth noting that high stresses occur not only in the immediate neighborhood of the shear bands but also at a distance from them. As a result, new shear bands (or cracks) can form in these regions.

The distribution of impurities near the polysynthetic shear band is found from the relation [5]

$$C = C_0 \exp\left(-U/(kT)\right),$$

where C_0 is the impurity concentration far from the internal stress sources, k is the Boltzmann constant, and T is the absolute temperature. The energy U of interaction between the impurity and polysynthetic shear band has the form

$$U = -(4/3)\pi r^3 \varepsilon (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}),$$

where r is the atomic radius of the matrix, $\varepsilon = (r_0 - r)/r$ is a small parameter, r_0 is the atomic radius of the impurity, and σ_{xx} , σ_{yy} , and σ_{zz} are the normal stresses determined from relations (1).

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Fig. 2. Schematic of polysynthetic shear bands.



Fig. 3. Configurations of the stress fields near the polysynthetic shear band for $d = 0.2 \ \mu\text{m}$, $l = 2 \ \mu\text{m}$, $h = 1 \ \mu\text{m}$, M = 4, N = 10, and K = 3: a) $\sigma_{xx} = \sigma_{xx}(x, y)$; b) $\sigma_{xy} = \sigma_{xy}(x, y)$; c) $\sigma_{yy} = \sigma_{yy}(x, y)$; d) $\sigma_{zz} = \sigma_{zz}(x, y)$.



Fig. 4. Distribution of impurities near the polysynthetic shear band.

Figure 4 shows the calculation results. The calculations were performed for the binary Fe–B alloy characterized by the atomic ratio Fe : B = 0.75 : 0.25 for $b = 2.87 \cdot 10^{-10}$ m, $\mu = 0.168$, $\nu = 0.33$, $r = 1.27 \cdot 10^{-10}$ m, $r_0 = 0.97 \cdot 10^{-10}$ m, $k = 1.38 \cdot 10^{-23}$ J/K, and T = 300 K. The other parameters are the same as in Fig. 3. An important calculation result is that the maximum concentration of impurities occurs at a distance from the polysynthetic band rather than in the central part of the band (Fig. 4).

In summary, a dislocation model of a polysynthetic shear band, which often occurs in an amorphous material upon its deformation, has been proposed. Analytical expressions for stress fields and the distribution of impurities near a polysynthetic shear band in an amorphous material have been obtained. It has been found that both stresses and impurities are localized at a certain distance from the geometric center of the polysynthetic band.

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