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Modelling of plastic behaviour of compound semiconductors; from simple glide to multiglide

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Abstract

The compressive stress–strain curves of GaAs are simulated using a proposed model of multislip taking into account perfect dislocations of three types. The results show the dominant activation of dislocations by the primary slip system and the minor role of the secondary system. The yield drop observed at higher temperatures is not obtained. Possible applications of and existing restrictions on the model are mentioned.

1. Introduction

The progress in experimental techniques in recent years has enabled the performance of compressive tests on elemental and compound semiconductors under confining pressure at very low temperatures [1, 2]. The data obtained have contributed to the discussions of the plastic deformation mechanisms and a possible transition at high applied stress between the dissociated glide and the perfect undissociated dislocation configuration. Because of the simple form of the stress tensor, compression experiments are appropriate for testing dislocation dynamics models. Already published models operate with one [3, 4] or two [5] active slip systems. The need for a simulation of more complicated experiments performed on fcc-based compound semiconductors calls for a model with a greater number of active slip systems. In particular, the aim is to obtain the constitutive laws making it possible to describe the plastic behaviour of GaAs crystals indented at room temperature. The present paper proposes a model inspired by the generalized constitutive laws for fcc single crystals [6]. A simulation of uniaxial compression tests performed on GaAs single crystals at medium temperatures is presented and the properties of the model are discussed.

2. Model

The plastic deformation is caused by dislocation glide on the well-defined lattice planes characterized by the dislocation Burgers vector $\vec{b}^{(j)}$ and the normal vector of the glide plane $\vec{n}^{(j)}$, $j = 1, \ldots, 12$. The model consists of the equations describing the plastic flow, the evolution of dislocation densities in each system, and the internal stress. From the existence of two types of atom in compound semiconductors it follows that the perfect dislocation glide loops consist of segments with different core structures. Three types of dislocation (α, β, and screw) with different mobilities are thus distinguished and taken into account in the model.

The multislip model is based on the formalism of Alexander and Haasen [7]. The extension to multislip is achieved by modification of the form of the effective shear stress τ_{eff}. The expression $\tau_{\text{eff}}/\tau_0 = (\tau - \tau_\mu)/\tau_0$ used in the single-slip model of Alexander and Haasen is replaced by

$$\frac{\tau_{\text{eff}}}{\tau_0} = \frac{\tau^{(j)}}{\tau_\mu^{(j)}}, \tag{1}$$

where $\tau^{(j)}$ is the applied resolved shear stress on the jth slip system, and τ_0 equals 1 MPa. The internal stress τ_μ is dependent on the local dislocation densities in each system:

$$\tau_\mu^{(j)} = \frac{Gb}{2\pi(1-\nu)}\left(h^{\text{p}}\rho^{(j)} + h^{\text{f}}\sum_{k=1,k\neq j}^{12}\rho^{(k)}\right)^{1/2}, \qquad \rho^{(j)} = \rho_\alpha^{(j)} + \rho_\beta^{(j)} + \rho_s^{(j)} \tag{2}$$

with G being the shear modulus, ν the Poisson ratio of the material, b the magnitude of the Burgers vector. For simplicity, only two hardening coefficients are used: the self-hardening coefficient h^{p} and the latent hardening coefficient h^{f}. Moreover, the possibly different contributions of each type of dislocation to the hardening are not distinguished.

The laws for the velocity of individual dislocations deduced from experiments are

$$v_\alpha^{(j)} = V_{0\alpha}\left(\frac{\tau_{\text{eff}}^{(j)}}{\tau_0}\right)^{m_\alpha}\exp(-Q_\alpha/kT), \tag{3}$$

$$v_\beta^{(j)} = V_{0\beta}\left(\frac{\tau_{\text{eff}}^{(j)}}{\tau_0}\right)^{m_\beta}\exp(-Q_\beta/kT), \tag{4}$$

$$v_{\text{s}}^{(j)} = V_{0\text{s}}\left(\frac{\tau_{\text{eff}}^{(j)}}{\tau_0}\right)^{m_{\text{s}}}\exp(-Q_{\text{s}}/kT). \tag{5}$$

The different mobilities for the different types of dislocation are expressed by the pre-exponential factors $V_{0_{\text{i}}}$, the exponents m_{i}, and the activation energies Q_{i}; k is Boltzmann's constant, T the absolute temperature.

To obtain the flow law, we consider that to a good approximation only screw dislocations contribute to the plastic deformation in each glide system [8]. This assumption is based on the geometry of the perfect dislocation glide loops and the different mobilities of the different segments. Glide of dislocations on a system (j) is activated when the applied resolved shear stress $\tau^{(j)}$ is higher than the internal stress $\tau_\mu^{(j)}$. The strain rate is computed according to the Orowan relation with the use of the equation (5):

$$\dot{\gamma}_{\text{pl}}^{(j)} = 2\rho_{\text{s}}^{(j)}b_{\text{s}}v_{\text{s}}^{(j)} = 2V_{0\text{s}}\rho_{\text{s}}^{(j)}b_{\text{s}}\exp(-Q_{\text{s}}/kT)\left(\frac{\tau^{(j)}}{\tau_\mu^{(j)}}\right)^{m_{\text{s}}}. \tag{6}$$

The rate of the shear strain on the jth slip system $\dot{\gamma}^{(j)}$ consists of an elastic and a plastic strain rate:

$$\dot{\gamma}^{(j)} = \frac{\dot{\tau}^{(j)}}{\eta} + \dot{\gamma}_{\mathrm{pl}}^{(j)}, \tag{7}$$

with η the combined elastic modulus of the machine and the sample.

The model is completed by adding the law describing the evolution of each type of dislocation with strain for each slip system. The densities of α, β, and screw dislocations increase proportionally to each other [3]:

$$\dot{\rho}_{\mathrm{s}}^{(j)} = K_\alpha \rho_\alpha^{(j)} v_\alpha^{(j)} \frac{\tau_{\mathrm{eff}}^{(j)}}{\tau_0} + K_\beta \rho_\beta^{(j)} v_\beta^{(j)} \frac{\tau_{\mathrm{eff}}^{(j)}}{\tau_0} \tag{8}$$

$$\dot{\rho}_\alpha^{(j)} = \dot{\rho}_\beta^{(j)} = \frac{1}{2} K_{\mathrm{s}} \rho_{\mathrm{s}}^{(j)} v_{\mathrm{s}}^{(j)} \frac{\tau_{\mathrm{eff}}^{(j)}}{\tau_0}. \tag{9}$$

The multiplication constants K_{i} are not precisely known and, as a simplification, we use the same constant K for all three types of dislocation. Expressing $\rho_{\mathrm{s}}^{(j)}$ using equation (6) and substituting it into equation (9), we get

$$\dot{\rho}_\alpha^{(j)} = \dot{\rho}_\beta^{(j)} = \frac{K}{4b} \left(\frac{\tau^{(j)}}{\tau_\mu^{(j)}} \right) \dot{\gamma}_{\mathrm{pl}}^{(j)}. \tag{10}$$

From equations (6), (8), by simple algebraic manipulations, it follows that

$$\dot{\rho}_{\mathrm{s}}^{(j)} = \frac{K}{2V_{0\mathrm{s}} b_{\mathrm{s}} \exp(-Q_{\mathrm{s}}/kT)} \left[V_{0\alpha} \exp(-Q_\alpha/kT) \frac{\rho_\alpha^{(j)}}{\rho_s^{(j)}} \left(\frac{\tau^{(j)}}{\tau_\mu^{(j)}} \right)^{m_\alpha - m_{\mathrm{s}} + 1} + V_{0\beta} \exp(-Q_\beta/kT) \frac{\rho_\beta^{(j)}}{\rho_{\mathrm{s}}^{(j)}} \left(\frac{\tau^{(j)}}{\tau_\mu^{(j)}} \right)^{m_\beta - m_{\mathrm{s}} + 1} \right] \dot{\gamma}_{\mathrm{pl}}^{(j)}. \tag{11}$$

Other forms and modifications of the dislocation multiplication laws are possible. Tabourot *et al* [6] derived them from the balance between accumulation and annihilation rates of dislocation densities (annihilation is not taken into account here). They used the interaction matrix to express the mutual influences of different glide systems on the dislocation evolution. Our suggestion expressed by equations (10) and (11) results from our endeavouring to remain close to the successful model of Alexander and Haasen [7] and to use a form which is more convenient for multislip simulations.

3. Compression tests

The multislip model has been tested by simulation of the GaAs stress–strain curves obtained during compression tests along the $[\bar{1}23]$ axis with the compressional strain rate $\dot{\varepsilon} = 5.6 \times 10^{-5}\ \mathrm{s}^{-1}$. The Schmid factors for the most highly stressed systems are 0.47, 0.35, and 0.29. The experimental results are those described in [1].

The calculations were performed with the following material parameters: $G = 48$ GPa, $\nu = 0.33$, $b = 0.4$ nm. As the individual dislocation velocity parameters, we use the measured values of [9] summarized in table 1. All 12 slip systems are taken into account.

The hardening coefficients are chosen as $h^{\mathrm{p}} = 0.01$, $h^{\mathrm{f}} = 0.16$. Their values have been selected on the basis of the structural similarity with metals, without deeper physical justification. The initial total dislocation density in each system is $\rho_0 = 20 \times 10^{10}\ \mathrm{m}^{-2}$. The dislocation multiplication parameter K has to be adjusted. In an ideal case, when all other parameters are well chosen, $K = 1$. In the model presented, K is used as a fitting parameter.

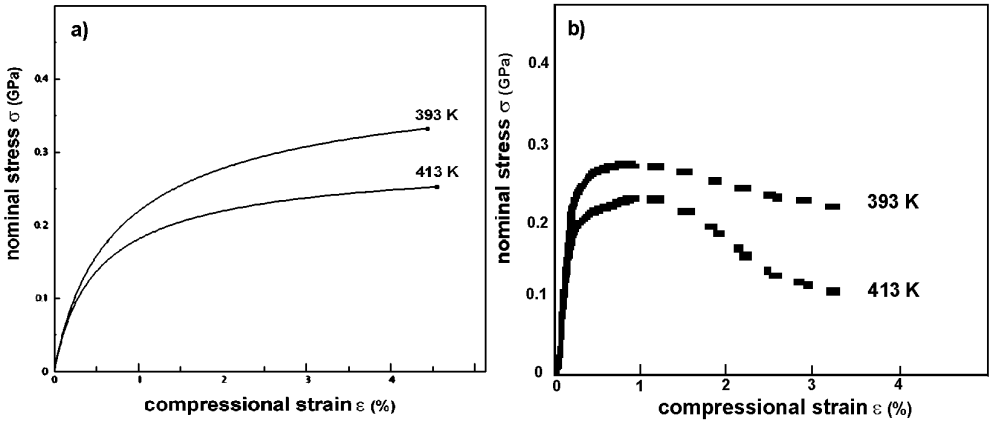

Figure 1. Calculated stress–strain curves for GaAs, for compressive deformation along the $[\bar{1}23]$ axis at a compressional strain rate of 5.6×10^{-5} m s^{-1} (a) and the corresponding schematic experimental curves according to [1] (b).

Table 1. GaAs dislocation velocity law values [9].

	α	β	Screw
Q (eV)	1	1.7	1.72
V_0 (m s^{-1})	900	8×10^4	9×10^5
m	1.7	1.7	2

The parameter η is adjusted using the initial part of the stress–strain curve, as it determines the slope of the elastic part.

The calculated compressional strain versus nominal stress dependence for the primary system $(1/2)[10\bar{1}](111)$ for temperatures $T = 393, 413$ K are shown in figure 1 together with experimental results from [1].

In the case of $T = 413$ K the parameter $K = 1.6\,\mathrm{m}^{-1}$, which indicates that the dislocation multiplication is a little amplified. The value $K = 1$ can probably be reached with other hardening factors. In contrast, for the temperature $T = 393$ K the dislocation multiplication was decelerated, by taking $K = 0.3\ \mathrm{m}^{-1}$.

The model presented does not allow one to obtain the yield drop characteristic for the higher-temperature stress–strain curves. The plastic part of the calculated curves has a parabolic shape typical for curves measured below 300 K [1]. This is caused by the form of the effective stress used in equation (1). Consequently, the model is suitable for describing the plastic properties at medium temperatures up to 1% of deformation and, in particular, at temperatures below 300 K. However, at low temperatures there is a lack of experimental dislocation dynamics data. Activation energies of dislocations are measured in the low-stress/high-temperature domain and are not applicable for low temperatures [4]. This is also why we present the calculated curves for only two temperatures. They have been found to be the most suitable to demonstrate the capabilities of the model.

The evolution of the total dislocation density in activated systems for $T = 413$ K in figure 2 shows, as expected for this crystal orientation, the predominant role of the primary system. It can be seen that the secondary system is also activated, but entirely in the early stages of deformation. The dislocation densities in the other systems remain practically constant.

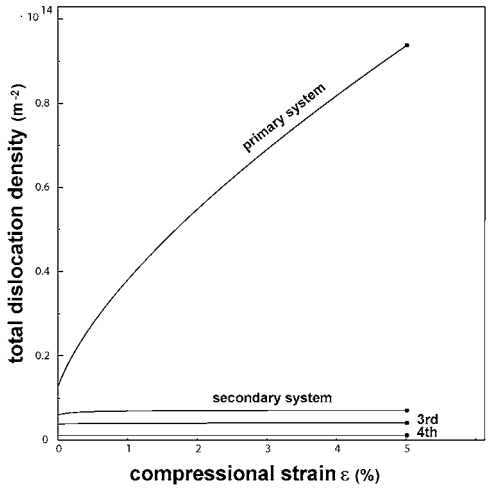

Figure 2. The calculated evolution of the total dislocation density, for each system, during the compression test at $T = 413$ K.

4. Conclusions

The suggested model represents an attempt to deal with multislip in the diamond-centred cubic compound semiconductors. The tests performed by modelling of the GaAs compressive stress–strain curves showed that with the form of the constitutive laws used the yield drop cannot be simulated. This restricts the applicability of the model to the early stages of deformation at medium temperatures and, in particular, to the range of low temperatures. The observed activation of two slip systems is obtained, confirming the dominant role of the primary slip system.

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