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Stress dependence of dislocation glide activation energy in single-crystal silicon-germanium alloys up to 2.6 GPa

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A new approach to the study of plastic flow in semiconductors is introduced. By analyzing relaxation of misfit strain in metastable strained-layer structures, the effects of resolved shear stress up to several GPa can be examined, at least an order of magnitude larger than is accessible using conventional loading techniques. This new approach is used to study stress-dependent dislocation dynamics in silicon-germanium crystals at resolved shear stresses as high as 2.6 GPa. The results are consistent with a conventional picture of dislocation dynamics which includes climb and glide processes, where the glide activation energy depends linearly on the applied stress.

I. INTRODUCTION

Plastic deformation in most solids is mediated by the thermally activated motion of dislocations. However, since there is a limit to the theoretical strength of materials, dislocation motion and plastic flow will occur even at zero temperature. There is a critical level of resolved shear stress, called the zero-temperature flow stress, at which the activation energy for dislocation motion becomes zero, and dislocation motion occurs spontaneously without thermal activation. This implies that the characteristic activation energies for dislocation motion in solids must be stress dependent, an effect well known in metals. Unfortunately, a similar statement cannot be made for semiconductors, in which the strong covalent binding produces zero-temperature flow stresses near 10 GPa. Mechanical loading experiments, which are typically limited by the onset of fracture to shear stresses in the 100-MPa region, reveal essentially no stress dependence of the dislocation mobility activation energy in semiconductors.[1] (There is some indication of stress dependence from microindentation experiments. In these experiments, however, the state of stress is not well defined, making quantitative studies difficult.) Nevertheless, at sufficiently high shear stress, dislocation mobility must become dependent on the applied stress. It is therefore of interest to develop new experimental techniques capable of studying this regime.

The purpose of the current paper is to introduce a new method for study of the stress dependence of dislocation mobility in semiconductors. This new procedure is based on experimental observations of strain relaxation in metastable strained-layer structures. These observations are then interpreted using a strained-layer relaxation model based on conventional plastic flow models for bulk semiconductors. (This model is related to recent kinetic models for relaxation of mismatch strain in such structures,[2,3] but is extended to include temperature-dependent effects, such as the transition from glide- to climb-dominated plastic flow, as well as stress-dependent activation energies.) This new method can be used to study dislocation dynamics and plastic flow in semiconductors with well-defined resolved shear stress as large as several GPa, extending the experimentally accessible regime by more than an order of magnitude in stress.

We apply this new procedure to the study of dislocation mobility in the Si-Ge system. Structures consisting of several hundred Å of single-crystal Si-Ge alloys were deposited coherently on a Ge(100) substrate. Dislocation glide activation energies were then extracted from the relaxation data for resolved shear stresses up to 2.6 GPa. These activation energies are found to be stress dependent, and the observed stress dependence is consistent with the behavior commonly observed in metals, where the dislocation glide activation energy depends linearly on the resolved shear stress.

In Sec. II dislocation glide and climb mechanisms are reviewed, and the stress dependence of glide activation energies in metals is briefly reviewed. In Sec. III the analogy between bulk deformation processes and the relaxation of mismatch strain in metastable semiconductor strained-layer structures is developed. Finally, in Sec. IV the temperature- and stress-dependent model for mismatch strain relaxation is developed. This model is applied to the experimental data to extract the stress dependence of the dislocation glide activation energy in this class of materials.

II. DISLOCATION DYNAMICS

At low temperatures ($T<0.5T_{\text{melt}}$ in semiconductors), dislocation dynamics is dominated by glide mechanisms. The velocity of dislocation glide in high-quality single crystals in which covalent bonding dominates is determined by the magnitude of the resolved shear stress driving dislocation motion relative to the Peierls lattice resistance.[4] The lattice presents an array of long, straight energy barriers (Peierls barriers) to the motion of a dislocation, forcing it to advance through nucleation of double kinks, which then separate under the influence of the applied stress.

When dislocation glide is limited by thermally activated nucleation of double kinks, the dislocation velocity can be written as a simple Arrhenius law

$$V=A\sigma^{m}\exp[-E_{\text{gl}}(\sigma)/kT]\ , \tag{1}$$

where V is the dislocation velocity, A is a material-dependent proportionality constant, σ is the resolved shear stress driving the dislocation motion, $E_{\rm gl}(\sigma)$ is the (stress-dependent) activation energy for dislocation glide, and T is the temperature. The coefficient m is near unity in silicon,[1] and the current discussion is not compromised by taking $m=1$, although this must be reevaluated when considering other semiconductors. The dislocation velocity can then be expressed as the product of a dislocation mobility and a driving force,

$$V=\alpha(\sigma,T)\sigma \ , \tag{2}$$

where the mobility

$$\alpha(\sigma,T)=C\exp[-E_{\rm gl}(\sigma)/kT]$$

depends on stress only through the activation energy.

At higher temperatures (perhaps $0.5-0.7T_{\rm melt}$ in the diamond-phase semiconductors), diffusion-mediated processes such as climb become important. In this regime, the combined effect of glide and climb processes can be approximated as the sums of the two relevant Arrhenius terms, so that the temperature dependence of the dislocation mobility is

$$\alpha(T,\sigma)=C_{\rm gl}\exp[-E_{\rm gl}(\sigma)/kT]+C_{\rm cl}\exp(-E_{\rm cl}/kT) \ , \tag{3}$$

where $C_{\rm gl\,(cl)}$ are the kinetic prefactors determining the relative importance of the glide (gl) and climb (cl) processes and $E_{\rm gl\,(cl)}$ represent the activation energies for glide or climb. Whereas the glide activation energy $E_{\rm gl}(\sigma)$ is expected to be strongly stress dependent, based on observations on metals, the activation energy for dislocation climb, which is essentially the activation energy for self-diffusion, is taken as independent of shear stress.

In metals, the activation energy for dislocation glide is known to decrease as the resolved shear stress increases. This stress dependence has been determined experimentally for resolved shear stress nearly up to the zero-temperature flow stress for many metals.[5] A phenomenological expression for this dependence is

$$E_{\rm gl}(\sigma)=E_0[1-(\sigma/\tau_0)^p]^q \ , \tag{4}$$

where E_0 is the glide activation energy at zero stress, and τ_0 is the zero-temperature flow stress. In most metals, $\tau_0<0.01\mu$, where μ is the shear modulus. The parameters p and q describe the shape of the Peierls barrier inhibiting dislocation motion. A simple square barrier would set $p=q=1$, but a better fit to the data on metals is provided by $p=\frac{3}{4}$ and $q=\frac{4}{3}$. This expression has been found to be useful for many metals.

The experimental status of stress-dependent dislocation mobility in semiconductors is not so clear. Many experiments have been carried out to evaluate the dislocation glide activation energy in diamond-phase semiconductors.[1,6] Except at very low stress, the glide activation energy is independent of stress up to the largest shear stresses (roughly 100 MPa) that have been examined with bulk-loading techniques. (Examination at larger stresses is generally ruled out by onset of brittle fracture in the sample.) This is perhaps not surprising, as the scale for stress-related effects is the zero-temperature flow strength, which microindentation experiments indicate is near 0.1μ, or about 6 GPa, in these materials.[5] Previous experiments have been limited to about 0.002μ, at which level the change in activation energy predicted by Eq. (4) would be similar to the uncertainty in the experimental results.

III. PLASTIC FLOW IN METASTABLE STRAINED-LAYER STRUCTURES

We propose to study the stress-dependence of the dislocation glide activation energy in semiconductors by examining the kinetics of strain relaxation in strained-layer structures. There is a great deal of evidence that strain relaxation is sluggish enough that complete relaxation does not occur on experimental time scales. In a recent paper,[2] we have demonstrated that the relaxation behavior of metastable semiconductor strained-layer structures can be semiquantatively described using a phenomenological model based on the treatment of Haasen and coworkers[1] of plastic flow in bulk diamond-phase semiconductors. This relaxation model will be extended to determine the stress dependence of dislocation glide activation energies based on experimental studies of strain relaxation.

The strain relaxation model introduced in Ref. 2 describes the relaxation of strained-layer structures in terms of plastic flow resulting from the combined effects of thermally activated dislocation glide [Eq. (1)] and dislocation multiplication. Although the mechanisms resulting in dislocation multiplication are not well understood, an empirical description is provided by fitting to experiments in which the dislocation density increases by orders of magnitude in the early stages of plastic flow of a high-quality bulk semiconductor crystal. These two effects then combine to provide an accurate description of plastic flow in a strained-layer semiconductor. In this model, climb processes were ignored, as was the stress dependence of the glide activation energy. That reasonable fits to the experimental data were still achieved is because the experiments were performed at a fixed temperature, where the nearly constant climb and stress contributions could be approximately included in a phenomenological prefactor.

Strain relaxation in a strained-layer structure is driven by the stress acting on threading dislocations in the strained overlayer. Since no stress field acts on the portion of the dislocation lying in the substrate, motion in the strained overlayer can only take place by elongation along the overlayer-substrate interface, resulting in production of a misfit dislocation. Such elongation is opposed by the line tension of the misfit dislocation, which acts as an effective stress retarding plastic flow. The difference between these two stresses is the excess stress which drives dislocation motion, and hence strain relaxation via plastic flow, in strained-layer structures. For a strained overlayer, the excess stress is

$$\sigma_{\mathrm{ex}}=\frac{2(1+\nu)}{(1-\nu)}\mu\epsilon-\frac{\mu(1-\nu\cos^2\beta)}{2\pi(1-\nu)}\frac{\ln(4h/b)}{(h/b)}\ , \quad (5)$$

where ν is the Poisson ratio, ϵ is the strain in the overlayer, h is the overlayer thickness, b is the magnitude of the Burgers vector, and β describes the orientation of the dislocation.

In our original model,[2] the time dependence of the strain relaxation γ can be described by a single nonlinear ordinary differential equation

$$d\gamma/dt=K(\sigma_{\mathrm{ex}},T)[\sigma_{\mathrm{ex}}(\gamma)/\mu]^2(\gamma+\gamma_0)\ , \quad (6)$$

where K is the product of the dislocation glide mobility α [Eq. (2)] with a stress-independent activation energy and a phenomenological constant describing the process of dislocation multiplication. Since the strained-layer structures are initially coherent and nearly dislocation free when properly grown, it is necessary to introduce a term γ_0 representing a source of dislocations. Such a term is physically reasonable, since even dislocation-free semiconductors are observed to have such sources which are active at rather low shear stress.[7]

The description of strain relaxation in semiconductor strained-layer structures provided by the above model was first applied[2] to a series of experimental measurements of strain relaxation in metastable Si-Ge/Si[100] structures studied by Bean and co-workers.[8] These films were grown at a substrate temperature of 550 °C over a broad range of film thickness and alloy composition. A comparison of the relaxation model with the Si-Ge strain relaxation data appears in Fig. 1. It is clear that the general trends of the relaxation process are accurately described by the present phenomenological model.

If this simple model is applied to a series of similar structures grown over a wide range of temperatures, however, the limitations of the model become apparent. Recent experiments by Tsao *et al.*[3] involved growth of a series of Si-Ge overlayers on Ge(100) substrates at temperatures ranging from 395 to 600 °C. At any given temperature, these structures relax in qualitative agreement with the predictions of Eq. (6). However, when the extent of relaxation observed at different temperatures is considered, the above model differs dramatically from the experimental results [Fig. 2(a)]. In order to describe the temperature-dependent relaxation data of Tsao *et al.*, our original model must be extended to include climb mechanisms and stress-dependent activation energies.

IV. STRESS-DEPENDENT THERMALLY ACTIVATED DISLOCATION MOBILITY

In most experiments the extent of strain relaxation is not determined as a function of overlayer thickness and strain. Instead, the overlayer thickness resulting in detectable relaxation at a given lattice mismatch is determined. (Relaxation of one part in a thousand is detectable using most common diagnostics [x-ray diffraction, Raman, low-energy electron diffraction (LEED) etc.].) This is sometimes called the "metastable" critical thickness.

The measurement of metastable critical thickness is equivalent to determining the excess stress needed to drive a given amount of relaxation within the timescale of the experiment. The value of σ_{ex} corresponding to the metastable critical thickness is the critical excess stress for that substrate temperature, which to first order is independent of the lattice mismatch. The relaxation behavior of the Si-Ge structures can thus be summarized in a stability plot of critical excess stress versus reduced temperature T/T_{melt}.[3] Since these quantities also result from the plastic flow relaxation models, it is convenient to compare the model predictions with experiment on such a stability plot.

It is straightforward to extend the earlier form of the strain relaxation model [Eq. (6)] to include dislocation climb and stress-dependent dislocation mobilities. Climb mechanisms can be introduced by replacing the simple glide mobility defined by Eq. (2) with the combined glide

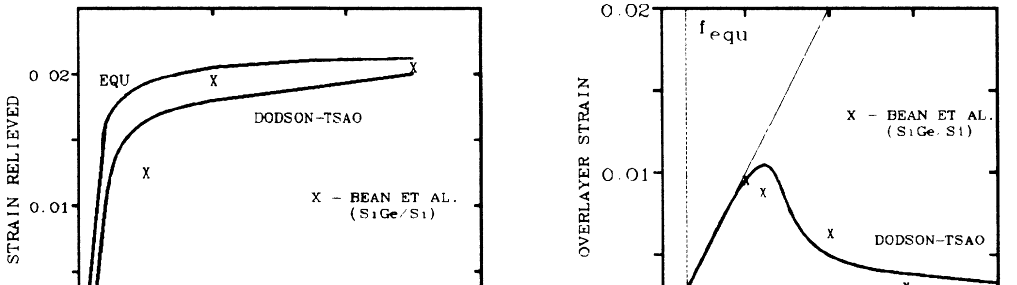

FIG. 1. Strain relaxation in metastable SiGe/Si[100] strained-layer structures. (a) Strain relaxation of $\mathrm{Si_{0.5}Ge_{0.5}}$ overlayers as a function of film thickness. (b) Residual overlayer strain of 500-Å SiGe overlayers as a function of lattice mismatch (as determined by overlayer composition). Experimental data (X) by Bean and co-workers (Ref. 8) in both cases are compared with an equilibrium model ($\sigma_{\mathrm{ex}}=0$) and our earlier kinetic model (Ref. 2). In (b), the vertical line indicates the equilibrium mismatch for a 500-Å film, and the sloped line corresponds to the case of no strain relaxation. The general trends of the kinetic model agree well with that of the experimental data.

and climb mobility from Eq. (3). The stress-dependent activation behavior is approximated, as discussed in Sec. II, by making the glide activation energy, but not the climb activation energy, depend on the stress in the overlayer. A further complication is that the experimental data represents alloys of various compositions, which may be expected to have different zero-stress activation energies. Fortunately, the scaled zero-stress activation energy $E(0)/kT_m$, where T_m is the melting temperature, is essentially constant over this alloy system. Using this relation, Eqs. (3) and (6) can be combined to give

$$\frac{d\gamma}{dt} = \Gamma\left(C_{gl} e^{-\Upsilon E_{gl}(\sigma_{ex})/kT_m} + C_{cl} e^{-\Upsilon E_{cl}/kT_m}\right) \times [\sigma_{ex}(\gamma)/\mu]^2(\gamma+\gamma_0)\ , \qquad (7)$$

where $\Upsilon = T_m/T$ and Γ is the (phenomenological) dislocation multiplication parameter. The relaxation model now depends only on the excess stress σ_{ex} and the reduced temperature Υ, and is easily compared to the experimental data for the entire alloy system. Measurements based on conventional loading experiments[1] indicate that $E_{gl}(0)/kT_m \approx 30$ for the Si-Ge alloy system. Reasonable variation of these numbers does not change the current discussion.

The crucial role of stress dependence of the glide activation energy on the observed critical stress values can easily be demonstrated. The temperature dependence of critical excess stress can be predicted within the model based on Eq. (7) under the assumption that the glide activation energy is stress independent. These predictions are compared to experiment in the stability diagram appearing in Fig. 2(a). The deviation of this stress-independent model from the experimental data clearly is large in the high-stress regime, showing that the stress dependence of the dislocation mobility is very significant in this regime.

It is possible to extract the stress dependence of the dislocation glide activation energy by fitting the relaxation model of Eq. (7) to the experimental data of Tsao *et al.* For this purpose, it is convenient (although not necessary) to choose a particular set of parameters for the phenomenological relation Eq. (4) for stress dependence of the dislocation glide activation energy. If the Peirels barrier blocking dislocation motion is square in cross section, the stress dependence of the glide activation energy is linear in σ, so that

$$E_{gl}(\sigma) = E_0(1-\sigma/\tau_0)\ , \qquad (8)$$

equivalent to Eq. (4) when $p = q = 1$. The values of p and q are determined by the detailed shape of the Peirels barrier. However, as the available data do not permit exact determination of these parameters, the linear dependence of Eq. (8) is assumed in the present discussion.

The model which results from Eqs. (7) and (8), with $E_{gl}(0) = 16kT_m$; $E_{cl} = 30kT_m$; $\tau_0 = 0.1\mu$; and $\gamma_0 = 10^{-4}$, is fit to the Si-Ge/Ge(100) data of Tsao *et al.* (The zero-stress activation energies are based on bulk plastic deformation experiments. The zero-temperature flow stress is an estimate based on microindentation experiments. The value of γ_0 is a nominal value based on our earlier relaxation model.[2] Reasonable variation of any of these parameter does not alter the conclusions of our present analysis.) The only unknown parameters in the resulting model are the preexponential constants ΓC_{gl} and ΓC_{cl}, which are varied until the predicted critical excess stresses agree with the experimental values. This strain relaxation model, with preexponential values of $\Gamma C_{gl} = 2 \times 10^{10}$ and $\Gamma C_{cl} = 3.0 \times 10^{21}$, provides a description of the temperature-dependent critical excess

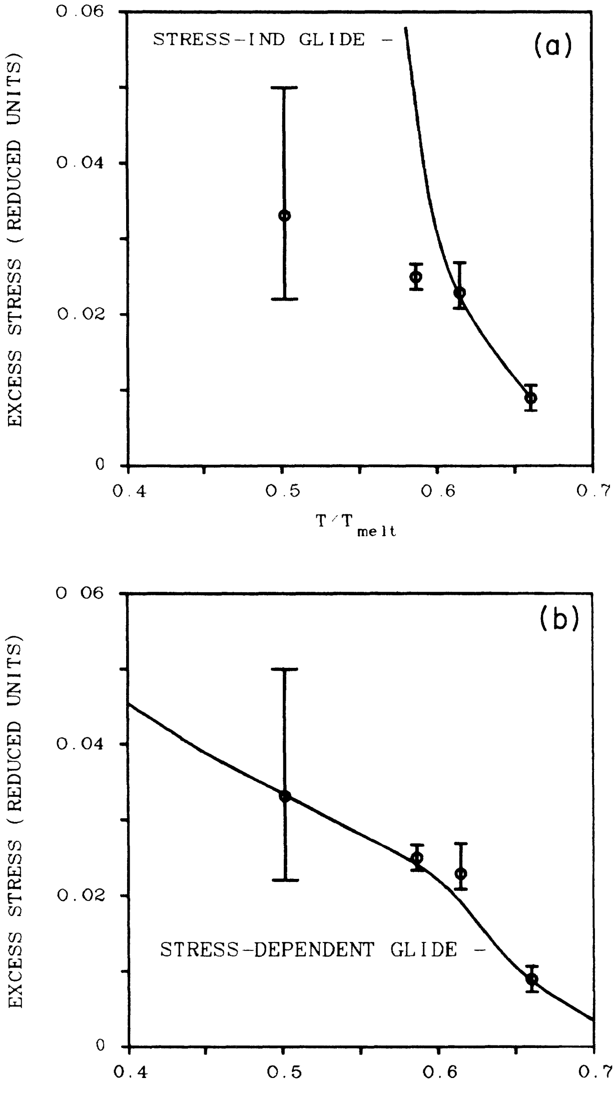

FIG. 2. Comparison of predictions of the phenomenological climb and glide model for plastic flow [Eq. (7)] developed in Sec. IV with the experimental data of Tsao *et al.* (Ref. 6) on "metastable" critical thickness. (a) Stress-independent dislocation glide activation energy; (b) stress-dependent activation energy [Eq. (8)]. The excess stress here is scaled by dividing by the shear modulus of the Si-Ge alloy. In (a) the assumption of stress-independent glide activation energy results in major discrepancies when compared to the experimental data at growth temperatures below $0.6T_m$. In (b) the inclusion of a simple description for stress dependence of the dislocation glide activation energy results in good agreement with the data.

stress consistent with the experimental data [Fig. 2(b)]. The value of $\Gamma C_{\rm gl}$ is fixed to within about 30% by requiring a good fit with the data, but $\Gamma C_{\rm cl}$ can vary by a factor of three or more without adversely affecting the resulting fit. (This is consistent with the relative magnitude of glide and climb processes in the temperature range under consideration.) There is, however, no basis for determining if the magnitudes of $\Gamma C_{\rm gl}$ and $\Gamma C_{\rm cl}$ are reasonable, as the roles of the dislocation mobility rate constants and dislocation multiplication cannot be separated in the context provided by the current experiments.

V. SUMMARY

In this paper we have outlined a new treatment of relaxation of misfit strain in metastable semiconductor strained-layer structures which applies over a large range of temperature and excess stress. This new framework makes possible the study of plastic flow in semiconductors under resolved shear stresses perhaps 20–30 times larger than those accessible using conventional loading techniques. This framework was then applied to study the stress dependence of dislocation dynamics in Si-Ge alloys at applied stresses up to 2.6 GPa. The experimental data are consistent with a conventional model including the effects of dislocation glide and climb, where the activation energy for dislocation glide depends linearly on the applied stress.

Note added. We recently received an unpublished report describing recent related work by R. Hull and coworkers. They have performed measurements of dislocation velocity and activation energy in strained Si-Ge structures using real-time transmission electron microscopy movies and a hot stage. for a pseudomorphic Si-Ge overlayer having 30% Ge, they measure a dislocation glide activation energy of 1.1 eV, compared to the bulk value of about 2 eV. This is in excellent agreement with the value of 1.03 eV predicted for this structure by the current model.

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