

Mechanical properties of undoped GaAs. Part I: Yield stress measurements

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Abstract

The present series of papers reports on the yield and fracture properties of undoped single crystal GaAs. In part I, the results of uniaxial compression tests over a range of temperatures, 200–550 °C, and strain rates, 2.5×10^{-5} – $2 \times 10^{-4} \text{ s}^{-1}$ are presented. Previous reports on deformation of GaAs have mostly involved tests in the ductile regime ($T \geq 400 \text{ °C}$). Although there are a few reports on low-temperature deformation tests in the brittle regime of GaAs, they were all performed in the presence of a hydrostatic pressure. The present experiments extend the deformations from the ductile to the brittle regime of the material without the superposition of a hydrostatic stress. In this way, the temperature- and strain rate dependence of the yield stress τ_y of GaAs has been determined. The results show an abrupt change in the deformation mechanism at a critical temperature T_{c2} that systematically increases with the strain rate $\dot{\epsilon}$. The critical temperature T_{c2} is in the same range as the brittle-to-ductile transition (BDT) temperature T_{BDT} of GaAs and follows the same trend with respect to changes in the strain rate. In part II of this series, we report on direct measurement of T_{BDT} of GaAs at different strain rates to see how it compares with the critical temperatures T_{c2} , obtained from uniaxial compression tests. For the measurements of T_{BDT} , we have used the technique of four-point bend testing. Finally, in part III, the same undoped GaAs material is deformed by static and dynamic (displacement-sensitive) indentation tests over a wide range of temperatures and the results compared with those obtained from compression experiments and four-point bend tests. The results show that the indentation BDT temperature T_{IBDT} is significantly lower than the value of T_{BDT} obtained from direct fracture experiments (part II), presumably because of the superimposed hydrostatic component present in an indentation. The microstructure of samples deformed by compression and indentation tests are also investigated by transmission electron microscopy and dislocation mechanisms are discussed to interpret the plastic and fracture properties of GaAs.

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1. Introduction

GaAs, like other compound cubic semiconductors, crystallizes in the zincblende structure (space group $F\bar{4}3m$), based on a face-centered cubic lattice with a basis of two atoms per lattice point at (0,0,0) and (1/4,1/4,1/4). Consequently, the slip system of GaAs is $\langle 1\bar{1}0 \rangle \{111\}$ and the dislocations have a Burgers vector $\frac{a}{2} \langle 1\bar{1}0 \rangle$, where $a = 0.5653 \text{ nm}$ is the lattice parameter of GaAs at 300 K.

With a bandgap of $\sim 1.4 \text{ eV}$ at room temperature – larger than that of silicon ($\sim 1.1 \text{ eV}$) – GaAs may be considered a moderate-bandgap semiconductor emitting in the red-orange part of the spectrum. It is one of the III–V compound semiconductors that has a direct bandgap and is thus widely used for the fabrication of optoelectronics devices. In fact, with the possible exception of hexagonal GaN, GaAs has probably received more attention than other direct bandgap semiconductors and its properties investigated in greater detail.

In addition to its direct bandgap, however, the mobility of electrons in GaAs is much superior to that of silicon

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($\sim 8500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ vs. $\sim 1500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for undoped crystals at 300 K) and this makes GaAs of considerable interest for high-frequency electronic device applications.

As with other semiconductors, lattice imperfections, and in particular line defects, are very detrimental to the electronic and optoelectronic properties of GaAs. Thus it is important to understand the conditions under which dislocations in GaAs are generated and the ease with which they glide. Also, since both generation and motion of dislocations are thermally activated processes, it is expected that there is a high-temperature limit to the use of GaAs for electronic applications. A good measure of the ease of generation of dislocations in any crystal is its yield stress τ_y , and a knowledge of the variation of τ_y with temperature, $\tau_y(T)$, provides a guide to the range of uses to which GaAs can be put in electronic devices. Moreover, the yield stress of semiconductors is known to be very sensitive to the loading rate – or the strain rate $\dot{\epsilon}$ – and to generally increase with an increase in $\dot{\epsilon}$. Thus, a full knowledge of $\tau(T, \dot{\epsilon})$ for any crystal requires measurement of the yield stress over a wide range of the two variables, temperature and strain rate.

In general, due to the brittleness of semiconductors at relatively low temperatures (below about $2/3T_m$), their yield stress has mostly been measured in the ductile regime of the material at temperatures above $2/3T_m$, where T_m is the melting point of the crystal in K. In the case of GaAs, there are a number of reports in the literature involving mechanical tests in the high-temperature range (400–800 °C) [1–5]. However, the reported data vary from one study to the other, are sometimes contradictory and often show large scatters. This arises partly from the different experimental techniques employed, the different orientations and types (nature and concentration of dopants) of GaAs crystal used, and the different range of temperatures and strain rates employed by the different investigators.

In this paper, we have used uniaxial compression tests at different temperatures and strain rates to measure the critical resolved shear (yield) stress τ_y of undoped GaAs and its temperature and strain rate dependence $\tau_y(T, \dot{\epsilon})$. The experiments were performed over the temperature and strain rate ranges 200–550 °C and 2.5×10^{-5} – $2 \times 10^{-4} \text{ s}^{-1}$, respectively, which covers both the brittle and the ductile regimes of GaAs. From the stress–strain plots at each temperature and strain rate, the critical resolved shear stress τ_y was determined. Two types of sample orientations were studied by this technique: one set of samples was oriented for single glide and the other for multiple glide. For both sample orientations, and the strain rates employed, the plot of $\ln(\tau_y)$ vs. $1/T$ showed a break at a critical temperature T_{c2} in the range 300–380 °C. From the experimental stress–strain data, the activation energy for dislocation glide was determined using two different methods. Finally, transmission electron microscopy was used to investigate the samples deformed at different temperatures. Below T_{c2} , the microstructure of deformed GaAs was found to be dominated by a low density of partial dislocations,

either as isolated leading partials each dragging a stacking fault, or as an array of leading partials on parallel adjacent planes forming microtwins. In contrast, for deformations at temperatures above T_{c2} , a high density of perfect dislocations, dissociated into leading/trailing partial dislocation pairs, were observed.

1.1. Low-temperature deformation of semiconductors

Plastic deformation of a semiconducting crystal with a low initial density of dislocations is not easy at low temperatures because the crystal is liable to fracture before it shears. To prevent the crystal from fracturing before yielding, two techniques are frequently employed. One technique involves two-stage deformation, where dislocations are first introduced in the crystal by pre-straining it at a high temperature (in the ductile regime) followed by lowering the temperature under load to the brittle regime and applying a high stress to move the dislocations and shear the crystal (see, e.g. Ref. [6]). The introduction of dislocations in the first stage prevents fracture under the high stresses that are required to shear the crystal at the low temperature of the second stage. The second technique involves direct deformation of the crystal at a low temperature (in the brittle regime) under a large shear stress in the presence of a superimposed hydrostatic pressure. The presence of the hydrostatic pressure counteracts the nucleation and propagation of microcracks and suppresses fracture by the tensile component of the high stress. Both types of experiments are rather involved and in the case of the second technique requires specialized facilities that enable the superimposition of a hydrostatic pressure on the applied shear stress. In the case of GaAs, Demenet et al. [7] and Boivin et al. [8] performed such experiments using a Griggs machine and made an extensive study of dislocation formation in the material. More recently, Suzuki and collaborators [9–12] used the same technique to plastically deform GaAs and three other compound cubic semiconductors at much lower temperatures and found a hump in the yield stress vs. temperature plot. The deformation behavior of all four investigated crystals was very different above and below the hump. This is best observed when the $\tau_y(T)$ results are re-plotted as $\ln(\tau_y)$ vs. $1/T$, whereby the hump appears as a sharp critical temperature T_{c1} . In this form, the temperature variation of the yield stress appears as two straight lines, with the one at high temperatures ($T > T_{c1}$) having a much steeper slope than the one at low temperatures ($T < T_{c1}$). This same type of behavior was found by Samant [13] and Demenet et al. [14] in compression experiments on single crystal 4H- and 6H-SiC, this time without the superimposition of a hydrostatic pressure. Again, a plot of $\ln(\tau_y)$ vs. $1/T$ at each strain rate was found to consist of two straight lines of different slopes, separated at a critical temperature T_{c2} . We use the subscripts T_{c1} and T_{c2} , respectively, to refer to compression experiments performed in the presence and absence of an external hydrostatic pressure. It is noteworthy that in all the

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