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Mechanical properties of undoped GaAs. II: The brittle-to-ductile transition temperature

Shanling Wang, Pirouz Pirouz *

Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, OH 44106-7204, USA

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Abstract

In this second part of a series of papers on the mechanical properties of GaAs, direct determination of the brittle-to-ductile transition temperature T_{BDT} of the same crystal as that used for compression experiments (see part I) is reported. The experimental technique employed for this purpose is four-point bend testing of pre-cracked samples at different temperatures and strain rates. It is found that, as in other semiconductors, T_{BDT} of GaAs is sharp, and is very sensitive to and increases with the strain rate from 300 to 380 °C for the strain rate ranging from $\dot{\varepsilon} = 1 \times 10^{-6}$ s^{-1} to $\dot{\varepsilon} = 5 \times 10^{-5}$ s^{-1}. From the variations of T_{BDT} with the strain rate $\dot{\varepsilon}$, the activation enthalpy ΔH_d for dislocation glide in undoped GaAs was determined to be 1.36 ± 0.02 eV, a value very close to that reported for the slow β dislocations in such a crystal.

Keywords: Semiconductor compound; Bending test; Dislocation structure; GaAs

1. Introduction

As described in part I of this series [1], compression tests at various strain rates on undoped GaAs exhibit a critical temperature T_{c2} at which there is an abrupt change in the slope of the linear plot of $\ln(\tau_y)$ vs. $1/T$. We had already found a similar behavior for the wide bandgap semiconductor 4H–SiC, where the intriguing point emerged that the transition temperature T_{c2} in the plot of the yield stress τ_y vs. temperature T was in the same range as the brittle-to-ductile transition (BDT) temperature T_{BDT} in that semiconductor [2,3]. This observation was later verified by direct measurements of T_{BDT} of the same 4H–SiC crystals at different strain rates [4]. Based on these results, a new model for the occurrence of BDT in semiconductors, the magnitude of T_{BDT} and its dependence on the strain rate $\dot{\varepsilon}$ was proposed [5]. It would thus be interesting to investigate whether the T_{c2} in GaAs, measured in part I [1], also corresponds to the T_{BDT} of this material. To the authors' knowledge, except for the indirect measurements of Fujita et al. [6], there are no reports on direct determination of the brittle-to-ductile transition temperature and its strain rate dependence for this important semiconductor. For this purpose, the T_{BDT} of the same undoped GaAs crystal as that used in part I [1] has been measured at different strain rates using the technique of four-point bend testing [4,7]. Combining the results of this paper with the microstructural changes that were observed by transmission electron microscopy (TEM), an attempt is made to correlate the transition from brittleness to ductility to the changes that take place in the type and character of dislocations that control plastic deformation of GaAs in different temperature and stress regimes.

GaAs, like most other cubic compound semiconductors, has a zincblende structure based on a face-centered cubic lattice with a $\langle 110\rangle\{111\}$ slip system and a $\{110\}$ cleavage plane. Because of the polar nature of GaAs, there are two types of non-screw dislocations in the crystal, commonly known as α and β dislocations [8]. These are distinguished by the nature of the atoms constituting the terminating

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* Corresponding author.
E-mail address: pxp7@cwru.edu (P. Pirouz).

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edge of the extra half plane. Conventionally, for dislocations on the shuffle plane, if the edge consists of Ga atoms, the dislocation is labeled α [or Ga(s)], and if it consists of As atoms, it is labeled β [or As(s)] [9]; conversely, for dislocations on the glide plane, α and β dislocations would correspond to As(g) and Ga(g), respectively. There are many experimental results in the literature that indicate widely different mobilities for α and β dislocations in GaAs [10–13]. Since most mechanical properties of a crystal are strongly influenced by dislocation mobility, it would be expected that the polarity of GaAs would also affect its brittle-to-ductile transition behavior.

2. Experimental

The four-point bend technique of pre-cracked bar-shaped samples to measure the brittle-to-ductile transition temperature T_{BDT} was first employed by Samuels in silicon [7]. More recently, Zhang et al. [4] used this technique to measure T_{BDT} in 4H–SiC. For our four-point bend experiments on GaAs, two types of bar-shaped samples with different orientations were prepared, shown in Fig. 1a and b. These two sample types were chosen because in the sample orientation shown in Fig. 1a, β dislocations are expected to activate on inclined $(1\,1\,1)$ and $(\bar{1}\,\bar{1}\,1)$ slip planes when a $[1\,\bar{1}\,0]$ Knoop indent is made on the $(0\,0\,1)$ crystal face. Conversely, for the sample orientation in Fig. 1b, α dislocations are expected to be activated on inclined $(1\,1\,\bar{1})$ and $(\bar{1}\,1\,\bar{1})$ slip planes when a $[1\,1\,0]$ Knoop indent is made on the $(0\,0\,1)$ crystal face. The samples were in the form of $35 \times 3 \times 1\ \mathrm{mm}^3$ parallelepipeds and their orientation was such that the tensile stress on the $\{1\,1\,0\}$ cleavage plane is maximized while maintaining a reasonable resolved shear stress on the $\{1\,1\,1\}$ primary slip plane. Thus in one set of samples (Fig. 1a), the $35 \times 3\ \mathrm{mm}^2$ top and bottom faces of the sample were cut parallel to the $(0\,0\,1)$ plane, the $35 \times 1\ \mathrm{mm}^2$ side faces were parallel to the $(1\,\bar{1}\,0)$ plane and the $3 \times 1\ \mathrm{mm}^2$ end faces were parallel to the $(1\,1\,0)$ plane, while in the other set (Fig. 1b), the side faces were parallel to $(1\,1\,0)$ and the end faces were parallel to $(1\,\bar{1}\,0)$. The four-point bend jig and the cylindrical rollers were made from molybdenum (Fig. 2). The rollers were polished to give a surface finish comparable to that of the GaAs samples. In the tests, the inner and outer rollers of the jig were placed on the opposite $(0\,0\,1)$ faces of the sample; the bending arm d – given by half the difference between the outer and inner rollers $\frac{1}{2}(L-l)$ – was 10 mm. To convert the values of load and displacement into stress and strain, the equation given by Bruneau and Pratt [14] for an elastic beam in a four-point bending configuration was used. According to this equation, the normal stress σ_{app} applied to the $(1\,1\,0)$ end faces of the sample is given by

$$\sigma_{\mathrm{app}} = 3Pd/wh^2 \tag{1}$$

where P is the applied load in Newtons, and w and h are the width and thickness of the sample, respectively, in millimeters.

The strain rate in the central portion of the beam is

$$\dot{\varepsilon} = \frac{6h\dot{\delta}}{3l(L-l)+(L-l)^2+4h} \tag{2}$$

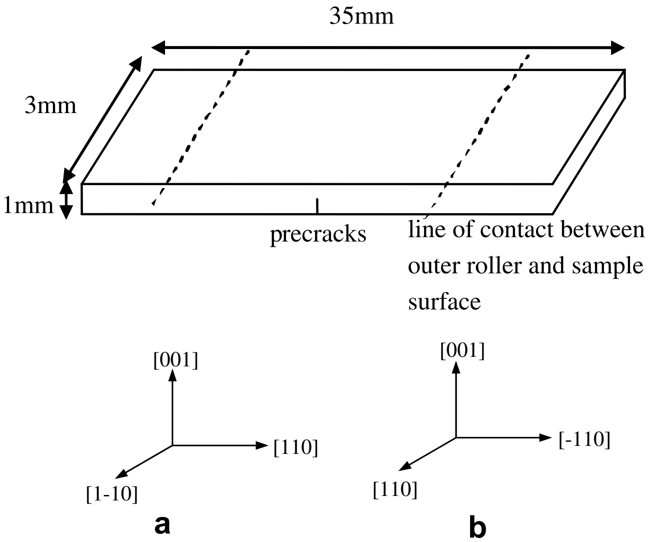

Fig. 1. Schematic of sample dimensions and orientations.

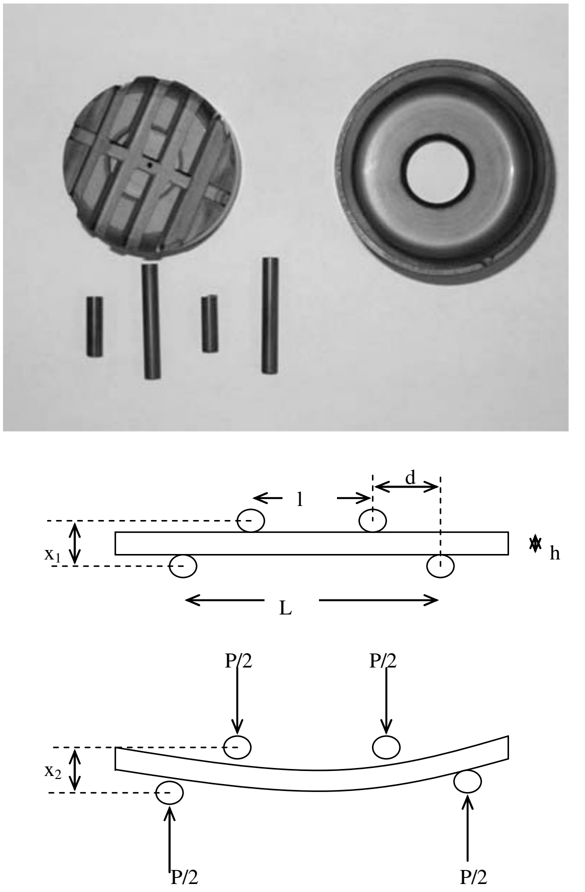

Fig. 2. Schematic of the four-point bending jig and geometry.