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Effects of Uniaxial Stress on the E_0'-Peak of Silicon

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ABSTRACT

Using the wavelength-modulation technique, we have measured the stress dependence of the E_0' peak of Si under uniaxial compression. The results suggest that the peak is a composite peak, with one part arising from transitions in the region around Δ (4-5) and the other part from transitions over an extended region around Γ.

Mit Hilfe der wellenlängen-modulations methode wurde die druckabhängigkeit des E_0' maximums in Si unter uniachsialem Druck gemessen. Die Ergebnisse legen die Folgerung nahe, dass das Maximum aus zwei komponenten zusammengesetzt ist, deren eine von Übergängen im Bereich um Δ (4-5) und deren andere von Übergängen in einem ausgedehneten Bereich um Γ herrührt.

The 3.45 eV reflection peak of Si has been the subject of controversy for sometime. From the dc piezoreflectivity measurements, Gerhardt[1] showed that the peak should have a Δ symmetry and is probably due to Δ (4-5) transitions near Γ. Results of experiments on chemical shifts of Ge-Si alloys,[2] ac piezoreflectance,[3] electroreflectance,[4] and piezo-electroreflectance[5] led to the same conclusion. On the other hand, similarity between the reflectivity spectra of the zincblende crystals[6,7] and their band structures[8] suggests that the peak might be due to Λ (4-5) transitions. Pseudopotential calculations of the deformation potentials of Si seem to support this latter assignment.[9] However, detailed band structure calculations indicate that an extended region of the Brillouin zone around the Γ point and around Δ and Λ axes is responsible for the observed peak.[8,10-13]

Recently, using the high-resolution wavelength-modulation technique, we were able to detect fine structure in this 3.45 eV peak of Si.[7,13] The spectrum suggests that the peak is a composite peak. Pseudopotential band calculations[13] identify the peak as due to transitions from a large volume around Γ,[14] and some extended region around the axes of Δ and Λ close to Γ. Comparison of the theoretical derivative spectrum with the experimental one shows surprisingly good agreement.[13] In order to obtain more information about this highly resolved composite peak, one would like to know how it varies under stress. In this note, we present results of our piezoreflectivity measurements on the 3.45 eV peak of Si using the wavelength-modulation technique. They indicate that the peak is probably due to transitions from the region around Δ and an extended region around Γ.

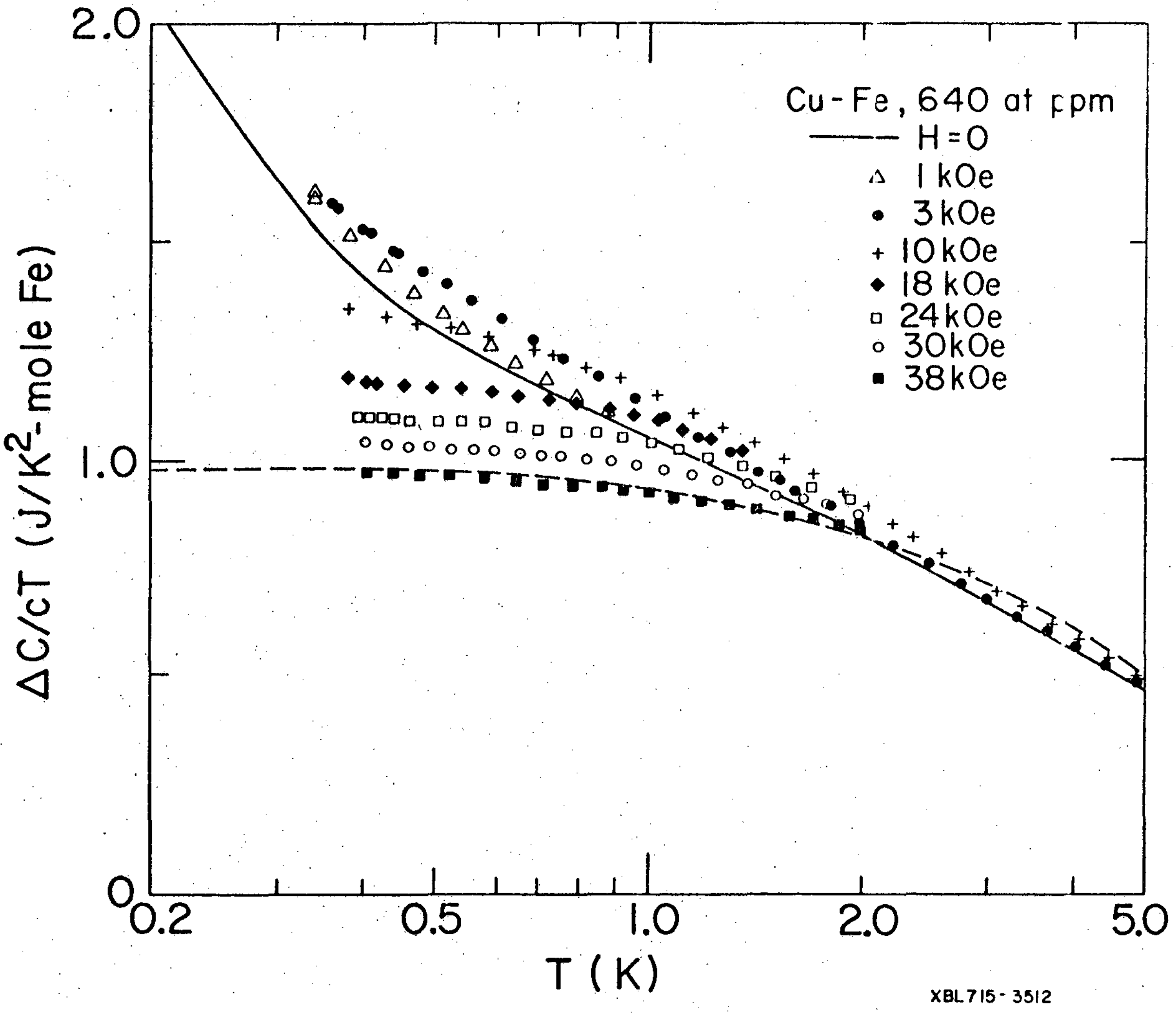
Cu-Fe, 640 at ppm
H=0
1 kOe
3 kOe
10 kOe
18 kOe
24 kOe
30 kOe
38 kOe
$\Delta C/cT$ (J/K^2-mole Fe)
2.0
1.0
0
0.2
0.5
1.0
2.0
5.0
T (K)
XBL715-3512

Fig. 3

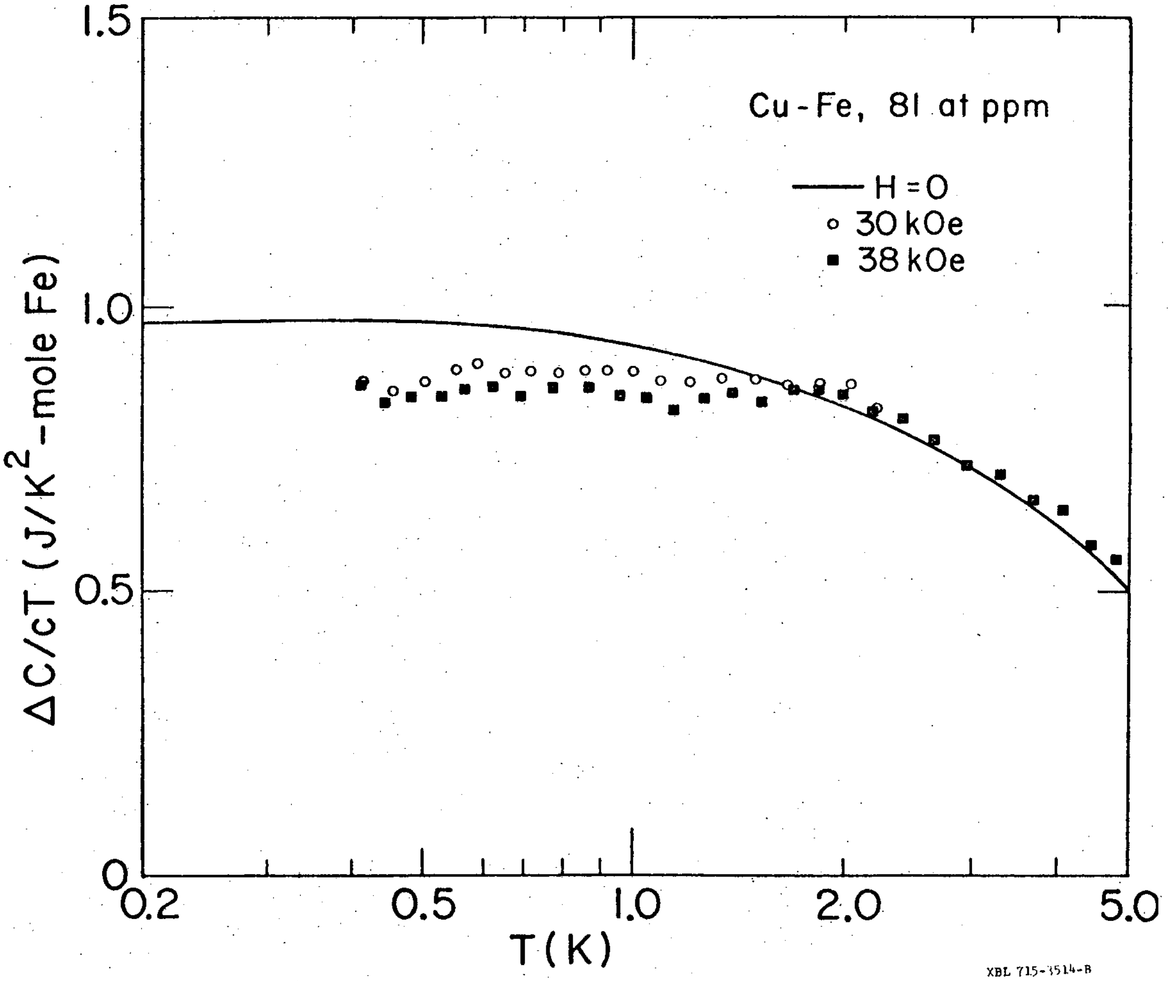

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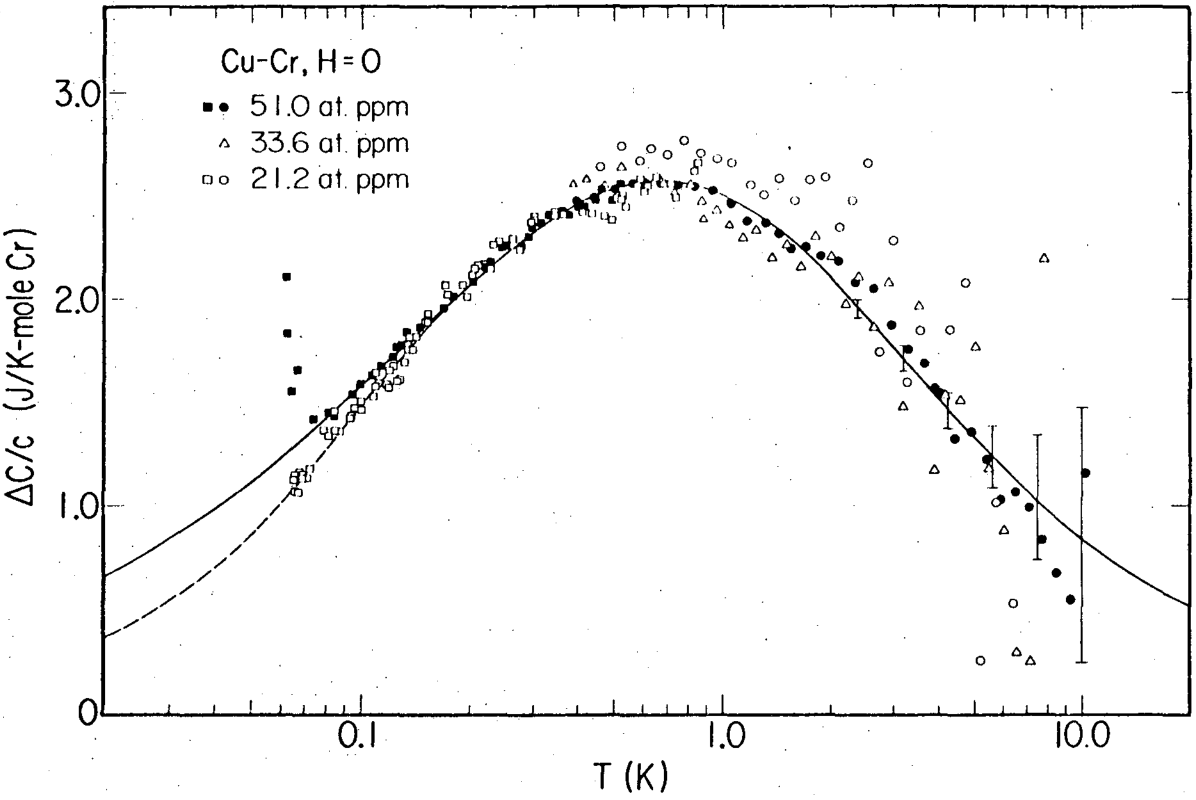
Fig. 2

Figure Captions

Fig. 1 The heat capacity of CuCr per mole of Cr. The solid curve represents the Bloomfield-Hamann theory, and the dashed curve is a linear extrapolation to T = 0. The error bars represent the effect of a 0.1% error in the total heat capacity.

Fig. 2 The heat capacity of 81 at ppm CuFe, per mole of Fe, as a function of magnetic field.

Fig. 3 The heat capacity of 640 at ppm CuFe per mole of Fe, as a function of magnetic field. The dashed curve represents the single-impurity zero-field behavior.



XBL 708-1976

Fig. 1

The wavelength-modulation spectrometer used for the measurements has been described elsewhere[7]. The stress apparatus was the same as that of Pollak and Cardona.[5] Two silicon crystals with dimensions 12 × 1.2 × 1.2 mm were cut and polished by Syton[15] before being mounted. One crystal had the long axis along [100] and the optical surface normal to [01$\bar{1}$]. The other crystal had the long axis along [111] and the optical surface normal to [1$\bar{1}$0]. The stress was always applied along the long axis of the crystal. Logarithmic derivative spectra $\Delta R/R\Delta E$ for reflectivity from normal incidence at $T = 10°K$ were taken with light polarization parallel and perpendicular to the stress axis.

Fig. 1a shows the spectra for zero stress and for stress $X = 5.5 \times 10^9$ dynes/cm^2 along the [100] axis. The obvious changes in the spectrum under stress are the shift of the zero point (corresponding to the maximum of the peak in the normal reflectivity spectrum) and the modification of the dip at 3.40 eV. With increasing stress, we found that for the spectrum with polarization parallel to [100], the zero shifted to lower energy and the dip gradually disappeared, and for the spectrum with polarization parallel to [011], the zero shifted to higher energy and the dip became somewhat more pronounced. This behavior can be understood if we assume that this 3.45 eV peak is composed of two superimposed broad peaks but slightly displaced from each other, and that the one which gives rise to the maximum in the normal reflectivity spectrum splits under stress while the other one does not. In Fig. 1b, the spectra with polarizations along [111] and [11$\bar{2}$] and for $X = 0$ and 11×10^9 dynes/cm^2 along [111] were shown. It is seen that for both polarizations, the spectrum under stress shows a small positive shift (~ + 0.017 eV and ~ 0.008 eV respectively) of the zero and a small reduction of the peaks (corresponding to a slight broadening of the peak in the normal spectrum).

The above results can be interpreted as follows. The composite peak is a superposition of two broad peaks. One centered at 3.45 eV is mainly due to transitions from the region around Δ (4-5), and has a dominant Δ symmetry. The other, centered at a slightly lower energy, is due to (4-5) transitions from an extended region around Γ and between Δ and Λ near Γ. The Δ peak would split into two under stress along [100], but would shift more or less as a whole under stress along [111].[16] The other peak should only broaden a little under stress since it is due to transitions from an extended region around Γ. No part in the peak seems to have a dominant Λ symmetry; otherwise, the spectra of the two polarizations would have shown clear difference under [111] stress.

In Fig. 2, the shift of the reflectivity maximum (or the zero of the derivative spectrum) is plotted as a function of stress for the four different combinations of stress direction and light polarization. The slopes (dE/dX) of the four curves are given in Table I.

Because of the complex nature of this composite peak, quantitative interpretation of the above results would be difficult. Calculations assuming only critical point transitions along directions of high symmetry are not likely to yield correct answers. However, a modification of the pseudopotential calculations treating the stress effects as perturbations can probably account for the detailed structure change of the peak under stress.

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14. The contribution to the peak from transitions around Γ was not explicitly stated in Ref. 13.

15. Product of Monsanto Chemical Co.

16. The observed small splitting in Fig. 1b may be due to the splitting of spin-orbit degeneracy which is often small compared with the shifts of critical points due to band distortion along equivalent directions under stress.

	Stress [100]		Stress [111]	
	Polarization [100]	Polarization [011]	Polarization [111]	Polarization [11$\bar{2}$]
$(\frac{dE}{dX}) \times 10^{-12}$ (eV-cm^2/dyne)	-2.4	+3.5	+0.7	+1.6

FIGURE CAPTIONS

Fig. 1. Wavelength modulation spectra of the E_0' reflectivity peak of Si under uniaxial compression.

(a) Stress $X = 5.5 \times 10^9$ dynes/cm^2 was applied along [100].

(b) Stress $X = 11 \times 10^9$ dynes/cm^2 was applied along [111].

In both figures, the solid curve is the spectrum obtained with zero stress, and the dashed curve and the dot-dashed curve are the spectra obtained under stress with light polarized parallel and perpendicular to the stress direction respectively.

Fig. 2. Shift of the maximum of the E_0' peak of Si as a function of the uniaxial stress for light polarized parallel and perpendicular to the two stress directions as indicated.

TABLE CAPTION

Table I. Stress coefficients of the E_0' peak of Si.

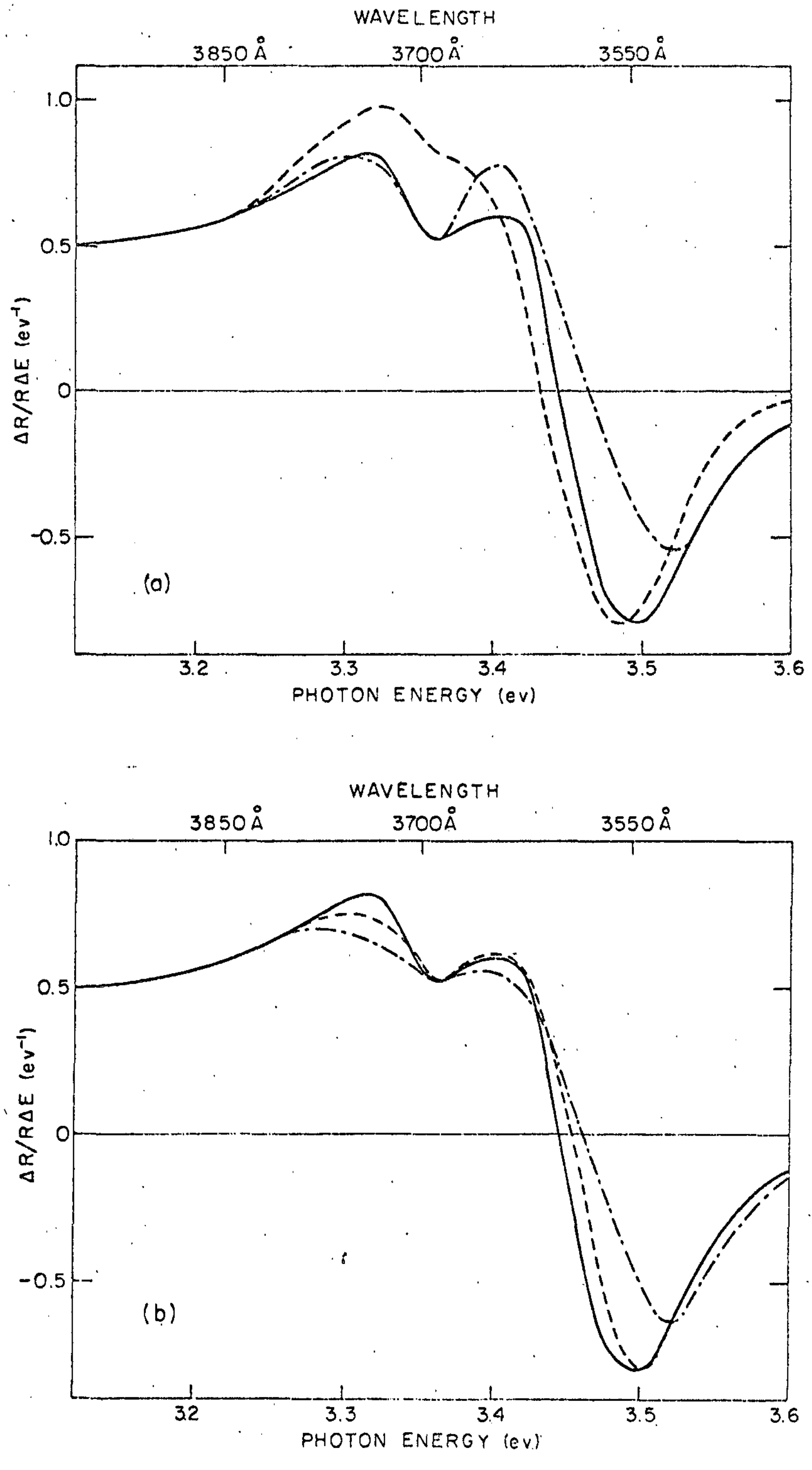

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Fig. 1

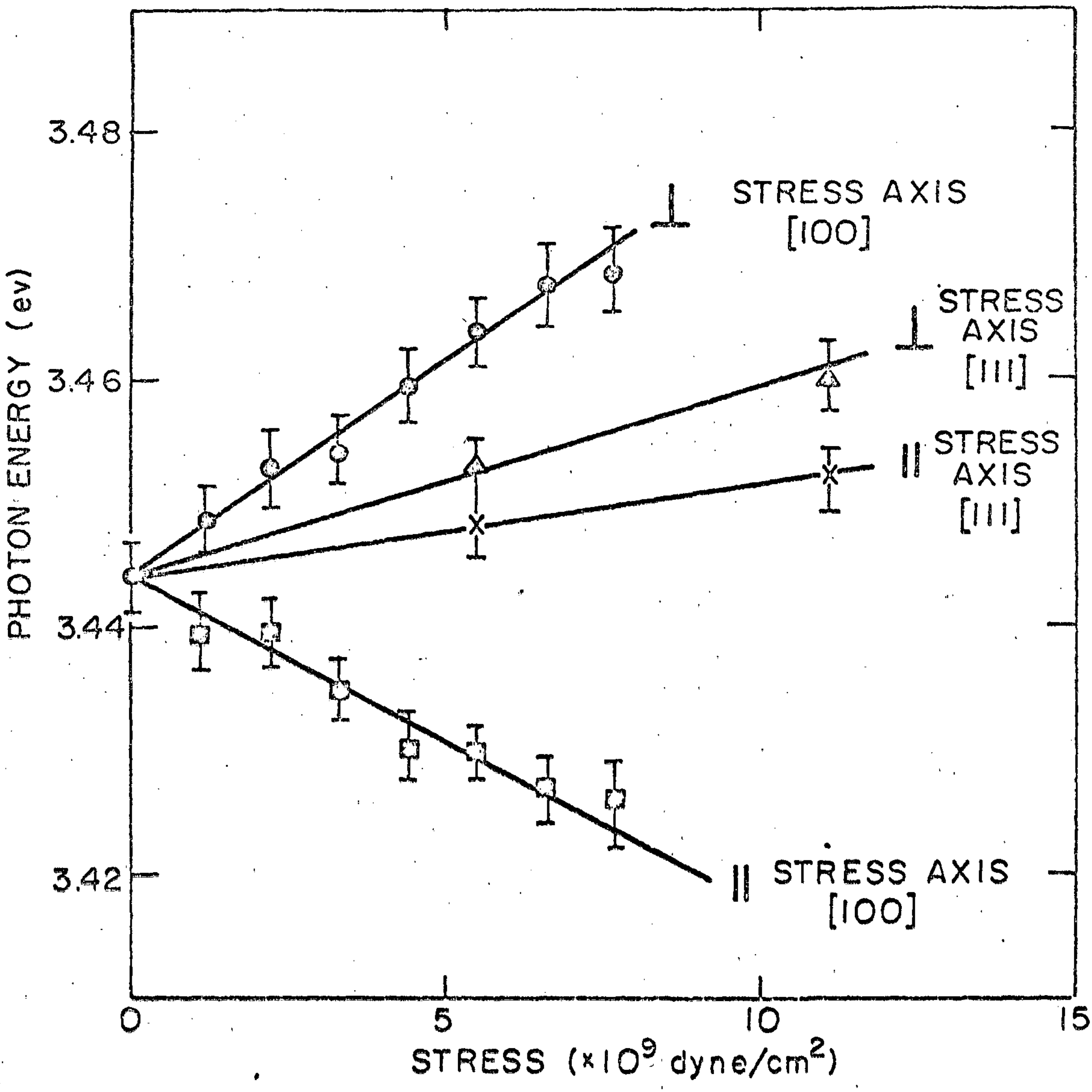

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Fig. 2

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