Comment on "New High-Pressure Transformation in a-Quartz"

In a recent Letter [1], Kingma et al. claim that the observed twinning in α -quartz recovered after pressurization provides an explanation for our previous report [2] of elastic anisotropy in this material. No support for this claim was offered by Kingma et al., and the estimates we present below show it to be untenable.

The effect of crystallites embedded in an elastically isotropic matrix on the sound velocities of the composite material depends upon the orientation of the crystallites. The maximum anisotropy would be produced if all the crystallites were to orient so that the directions of maximum and minimum velocity (7.0 and 5.3 km/sec, respectively) were to align exactly along the directions measured in our experiments. In this extreme case, 44% of the material would have to be crystalline in order to explain the anisotropy we measured. The directions of the velocity extrema in crystalline quartz have direction cosines $[0, 0.77, 0.64]$ and $[0, 0.94, -0.34]$ (referred to orthogonal axes) and are thus not orthogonal to one another, unlike our measurement directions. This taken together with the observed twinning and the fact that some of the crystallites retain their original orientation (thereby reducing the effect) implies that the actual fraction of crystalline material required to explain the observed elastic anisotropy must be considerably more than 44%.

An estimate of the amount of crystalline material can be obtained from Raman spectra. Spectra of fused $SiO₂$ and α -quartz recorded under identical experimental conditions show that the peak intensity of the 460 cm⁻¹ line of quartz is \sim 10 times more intense than the maximum in the spectra from fused $SiO₂$. Hence the spectra in

Refs. [1] and [3] lead to an estimate of \sim 10% crystalline material, and the spectrum in Ref. [2] (where no evidence of the crystalline peak is observed) gives $\lt 3\%$. These estimates are incompatible with the $>44\%$ required to explain the Brillouin results.

We conclude that although some of the material recovered when α -quartz is decompressed from pressures above 15-21 GPa may be crystalline, as stated by Kingma et al., this effect does not explain the observed elastic anisotropy in the recovered material. We still believe that the most likely explanation for the anisotropy is that the amorphous material produced in this manner is elastically anisotropic. We point out that, if true, this implies that the material is likely to be optically anisotropic as well. Caution should therefore be exercised in concluding that regions of a sample which do not produce extinction under crossed polarizers must be crystalline.

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