Binggeli and Chelikowsky Reply: In their Comment on our Letter [1], Chaplot and Sikka [2] suggest a "different conclusion" from ours with respect to the initiation mechanism for the pressure induced amorphization of α-quartz. They suggest that the initiation mechanism is a "soft *optic* phonon at the Brillouin zone boundary." This different conclusion of Chaplot and Sikka is without merit. Any distinction between two initiation modes separated in energy by a fraction of kT is questionable at best. Also, the local atomic displacement associated with the so-called soft "optic mode" is the *same* as that outlined in our Letter. The soft mode in question belongs to the *acoustic* branch, and is *not* an *optic* mode.

In providing a consistent physical description of the mechanism behind the quartz instability, we showed a connection between the softening of the acoustic branch and the packing of oxygens under pressure. We found that this softening was related to a change in the Si coordination from tetrahedral sites to octahedral sites in the oxygen sublattice.

The changes taking place in the acoustic branches between ambient pressure and 19 GPa are illustrated in Fig. 1. The flattening under pressure of the lowest acoustic branch extending from Γ is the softening process calculated in our Letter. *The lowest acoustic branch has an energy bandwidth expressed as a temperature of less than 50 K before any soft mode occurs.* The amorphization is observed experimentally, as well as in the simulations, at 300 K. Given this small bandwidth, one cannot focus on one single (zone edge) mode. When a transformation is first order, as it is in our case, it is clear that the transition *must* occur before any phonon or elastic instability occurs. Even for a weakly first order transition, the transition pressure can be several GPa below the instability of the elastic or phonon mode which triggers the transition [3]. Phonon dispersion curves alone cannot clarify the physical origin of the soft modes. We show in Fig. 2 the atomic displacements for the zone edge ($\mathbf{q}=\mathbf{K}$) phonon mode at 19 GPa. The Si atoms are clearly displaced from their tetrahedral sites to octahedral sites. Thus, the related local cation displacements and the *physical origin* of the acoustic branch softening, is the *same* as outlined in our Letter, namely a cation fourfold to sixfold site instability. This analysis confirms the conclusions of our Letter, which were based on the $\mathbf{q}\rightarrow 0$ behavior (soft shear).

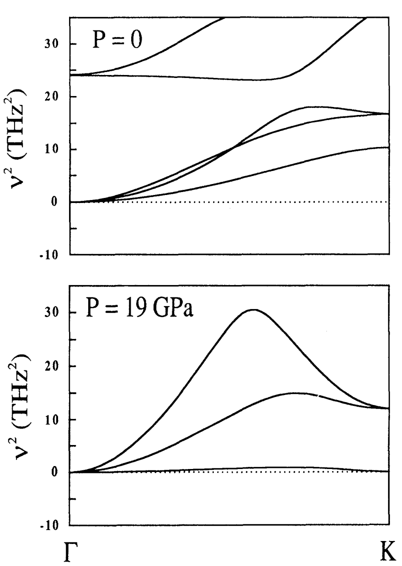

FIG. 1. Lowest phonon modes for α-quartz at ambient pressure and 19 GPa. The bandwidth of the lowest acoustic branch expressed as a temperature is less than 50 K at 19 GPa.

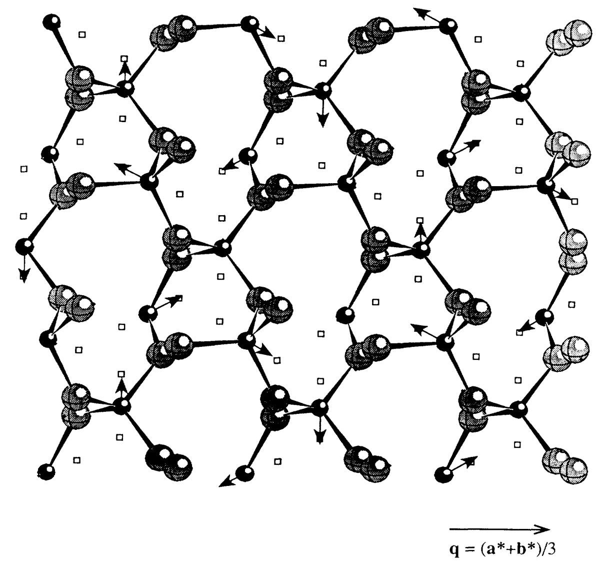

FIG. 2. Ball and stick model of α-quartz at 19 GPa. The arrows indicate the Si displacements for the *zone edge* mode. The open squares represent octahedral sites. The structural transformation is related to a coordination instability [1].

In short, the results of Chaplot and Sikka do not contradict the conclusions of our Letter. They simply reinforce our conclusions.

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