Theoretical Analysis of Elastic Softening in Diamond

T. Nakamura[1], T. Matsuzaki[1], Z. Huang[2], and N. Iwahara[1]

[1] *Department of Materials Science, Chiba University, Chiba, Japan*

[2] *Technische Universitat Berlin, Berlin, Germany*

Diamond becomes soft below 1 K. The shear elastic constant of diamond drops below 1 K (Figure 1). The contribution of neutral vacancies in diamond (Figure 2) has been predicted as the origin of this softening. However, the ground electronic state of a neutral vacancy in diamond is ^{1}E type and should not respond to shear strain (Γ_5).

In this work, we study if the neutral vacancies contribute to the elastic softening of diamond. To this end, we calculated the model Hamiltonian of neutral vacancy using DFT. The model consists of the Hund's rule vibronic coupling, and spin-orbit coupling. Then, we calculated the Helmholtz free energy using the model's energy eigenstates. Furthermore, the shear elastic constant $C_{44}(T)$ was obtained by numerically calculating $\partial^2 F / \partial e_{xy}^2$.

$C_{44}(T)$ obtained by the interaction calculation decreased below 1 K (Figure 3). This indicates that the ^{1}E state responds to Γ_5-type strain. However, the magnitude of this softening was approximately 1000 times smaller than the experimental data. The results suggest that the model used in this study alone cannot fully explain the significant response observed in the experiment.
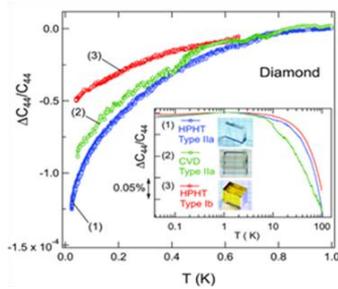

Figure 1. Temperature dependence of the shear elastic constant [1].
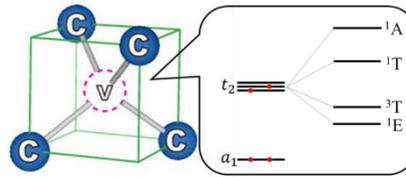

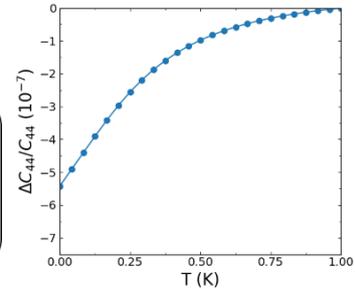Figure 2. Neutral single vacancy and defect levels in diamond [1,2].

Figure 3. Temperature dependence of the shear elastic constant calculated by DFT.

References

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