Sun *et al.* Reply: In the preceding Comment [1], Akola and Jones (AJ) claim that our findings [2] are artifacts of details of the simulations, particularly the fast cooling rate, relative small simulation cells, and periodic boundary conditions (PBC).

Many successful cases show that this claim of AJ is very subjective, for example, in the work on Ge [3] by authors of the VASP code, a cell of 64 atoms and a fast quenching rate of 1.67×10^{14} K s^{-1} as well PBC were used. But this work produced reliable results which agree well with the available experimental data. We should emphasize that in Ref. [2] we used a cell of 243 atoms as well as quenching rates of 6.6×10^{12} K s^{-1} (from 1000 to 300 K) and 3×10^{14} K s^{-1} (from 5000 to 1000 K). Another example is some previous work by two of the present authors [4], where an ensemble containing 32 atoms was used. We agree that cavitations would take place in the system upon rapid cooling under a constant volume with PBC. However, in the nitrogen doped $Ge_2Sb_2Te_5$ (GST) system of our recent work [5] wherein a similar density as that in Ref. [2] was used, such voids were not observed even though a smaller cell (120 atoms, with the same shape as in Ref. [2]) and a faster cooling rate were applied. But the results of [5] agree well with experimental results. In our previous work for $Ge_1Sb_2Te_4$ [6], where a cubic cell with 189 atoms plus 27 vacancy positions and the same *ab initio* molecular dynamics parameters as Ref. [2] was used, we also observed large vacancy clusters surrounded mainly by twofold and threefold coordinated Te atoms. Therefore, we believe that the present observed large vacancy clusters in molten GST225 are not artifacts of the simulations, the cooling rate or the cell size used in Ref. [2].

Second, AJ ignored one critical condition, i.e., the first minimum of $g(r)$ which determines the coordination numbers (CNs), when they criticized the larger values of CNs given in Ref. [2]. Because the minimums (r_m) of $g(r)$ are not sharply defined for the molten GST system, even a small change of r_m may fundamentally change the results. As seen in Table I of Ref. [1], even for the same system, AJ obtained quite different values. Therefore, it is meaningless just to talk about the absolute CN values without comparing the important parameters which have great effect on them. We would like to emphasize that in our previous work [7] where different cutoff distances were used, smaller values of CNs were obtained for liquid $Ge_2Sb_2Te_5$, for example, $Z_{Ge-Sb} = 0.12$, $Z_{Sb-Sb} = 0.25$, which are smaller than that listed in Table I of Ref. [1]. In Ref. [7], the values of Z_{Ge}, Z_{Sb}, and Z_{Te} are 3.75, 3.08, and 2.58, respectively, which agree well with all the references listed by AJ [2].

Finally, we would like to emphasize that Te atoms, vacancies, and phase transition in GST are not new long before the publications of Ref. [8]. In Ref. [2] we explicitly pointed out that the clustering of lower coordinated Te atoms results in the formation of large voids. To summarize, we do not see much rationale in the presented criticism of our work.

Zhimei Sun,[1,*] Jian Zhou,[1] Andreas Blomqvist,[2] Börje Johansson,[2] and Rajeev Ahuja[2]
[1]College of Materials
Xiamen University
361005 Xiamen, China
[2]Department of Physics and Materials Science
Condensed Matter Theory Group
Uppsala University
Box 530, 75121 Uppsala, Sweden

Received 29 May 2009; published 6 January 2010
DOI: 10.1103/PhysRevLett.104.019604
PACS numbers: 61.43.Dq, 61.43.Bn, 64.60.Cn, 71.15.Pd

*zmsun@xmu.edu.cn

[1] J. Akola and R. O. Jones, preceding Comment, Phys. Rev. Lett. **104**, 019603 (2010).
[2] Z. Sun, J. Zhou, A. Blomqvist, B. Johansson and R. Ahuja, Phys. Rev. Lett. **102**, 075504 (2009).
[3] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[4] A. B. Belonoshko, R. Ahuja, and B. Johansson, Phys. Rev. Lett. **84**, 3638 (2000); Nature (London) **424**, 1032 (2003).
[5] Z. M. Sun, J. Zhou, H. J. Shin, A. Blomqvist, and R. Ahuja, Appl. Phys. Lett. **93**, 241908 (2008).
[6] Z. M. Sun, J. Zhou, A. Blomqvist, B. Johansson, and R. Ahuja, Appl. Phys. Lett. **93**, 061913 (2008).
[7] Z. Sun, J. Zhou, and R. Ahuja, Phys. Rev. Lett. **98**, 055505 (2007).
[8] J. Akola and R. O. Jones, Phys. Rev. B **76**, 235201 (2007).

