Reply to ''Comment on 'Phase diagram of MgO from density-functional theory and molecular-dynamics simulations' ''

Alejandro Strachan, Tahir Çağın, and William A. Goddard III*
Materials and Process Simulation Center, Beckman Institute (139-74), California Institute of Technology, Pasadena, California 91125
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In answer to a Comment by Belonoshko [Phys. Rev. B **63**, 096101 (2001)], we show that the B1-liquid melting curve of MgO obtained using two-phase simulations is in good agreement with the published one obtained using the Clausius-Clapeyron equation in conjunction with separate single phase calculations of liquid and solid.

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The main point of the Comment by Belonoshko[1] regards the calculation of melting curves from molecular dynamics (MD) simulations. In our paper[2] we calculated the melting curve $T_m(P)$ by integrating the Clausius-Clapeyron (CC) equation ($dP/dT = 1/T\Delta H/\Delta V$), which relates the slope of the melting curve to the change in enthalpy and volume between the liquid and solid phases. The quantities ΔH and ΔV were calculated via MD simulations using the qMS-Q force field derived from quantum mechanical calculations. The ΔH and ΔV data were obtained by heating the solid well into the liquid region and then cooling the liquid well into the solid region, leading to a range of temperatures where both liquid and solid properties can be calculated. This integration method requires an integration constant to obtain absolute melting points. Thus we obtain a family of melting curves. We chose the starting point for the integration of the CC equation as $T = 3100$ K at $P = 0$, based on an estimate of overheating from our previous studies. We *estimated* the error in the melting temperature by starting the integration at $T = 3050$ K and $T = 3150$ K at $P = 0$.

Belonoshko[1] argues that two-phase simulations are more precise (since they directly provide the melting temperature) and less intensive computationally. We have previously used two-phase simulations to predict melting temperatures for metals, but the two-phase method leads to less precise temperature derivatives than the CC approach and the more important discrepancies between simulations and experiment regard the *slope* of the melting curve.

To illustrate the comparison between the two-phase and CC methods, we show in Fig. 1 the B1-liquid coexistence curve of MgO using in both cases the same qMS-Q FF. The two-phase results (circles in Fig. 1) agree very well with our previous calculations using the CC equation (line in Fig. 1).

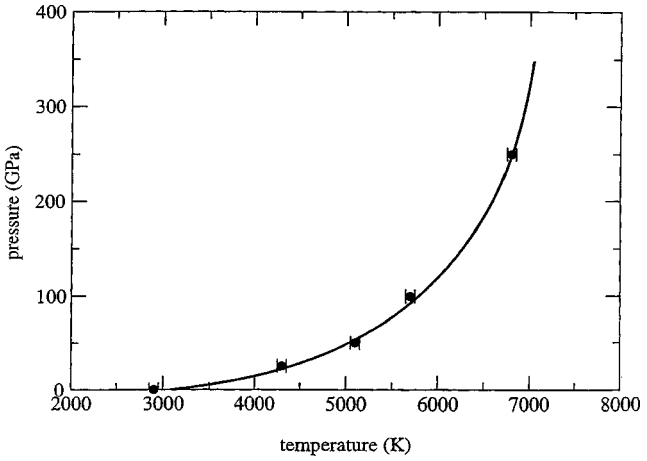

FIG. 1. B1-liquid coexistence curve of MgO obtained using the qMS-Q FF. Circles denote melting temperatures obtained using the two-phase method and the line shows the melting curve obtained using the Clausius-Clapeyron equation.

*Author to whom correspondence should be addressed.

[1] Anatoly B. Belonoshko, preceding Comment, Phys. Rev. B **63**, 096101 (2001).

[2] Alejandro Strachan, Tahir Çağın, and William A. Goddard, III, Phys. Rev. B **60**, 15 084 (1999).

