High Pressure Melting vs Decomposition of GaN: *ab initio* Molecular Dynamics Study and comparison to the experimental data

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Abstract ()

The technology of GaN is very much advanced due allowing for key applications like LEDs or high power-high frequency transistors. Nevertheless, GaN fundamental physical properties including phase diagram, are still not determined. In this work, simulations of GaN crystal behavior at heating to extremely high temperatures in a wide pressure range are reported. A*b initio* density functional theory (DFT) Molecular Dynamics extensive calculations were used to obtain the temporal change of the system. Heating of an initially perfect wurtzite GaN crystal to a temperature above 3500K resulted in destruction of the crystalline lattice and transition of the system to a perfectly disordered fluid. At the pressure of 7.1 GPa and below, the formation of N_2 molecules inside the cluster was detected, therefore the process was identified as the thermal decomposition of GaN. At pressures as high as 15 GPa, the formation of N_2 molecules was suppressed despite of total loss of the crystalline order. The system consisted of the single gallium and nitrogen atoms, so the high pressure process was identified as congruent melting of GaN.

An excellent agreement of the simulation results with well-established experimental data on GaN decomposition has been found. The absence of N_2 molecules in the fluid at high pressures indicates that the intersection of the decomposition line and the melting line occurs in the pressure range between 7 and 15 GPa. At pressure above the intersection point, gallium nitride can be congruently melted without decomposition in contrast to lower pressures where GaN decomposes before reaching the melting point. This is in agreement with the proposed melting model based on our earlier experiments, suggesting a reversal of the decomposition-melting sequence at heating, at 12 GPa.