MELTING BEHAVIOR OF GaN NANOWIRES : MOLECULAR DYNAMICS STUDY

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GaN is a promising semiconductor material that exhibits many outstanding physical and chemical properties in high-temperature, high-power, and high-frequency devices. One-dimensional GaN nanowires have also attracted much interest due to their significant potential for nanoscale electronics. Recently, many experimental investigations have been reported for the synthesis and the physical property of GaN nanowires [1,2]. In this paper, we investigate the structure and the melting behaviour of hexagonal GaN nanowires using the molecular dynamics (MD) simulations based on the Stillinger-Weber potential for GaN [3].

We first calculate the optimized structure of hexagonal GaN nanowires with the [0001] growth direction. Figure 1 shows the optimized structure of the GaN nanowire with the diameter of 28.67 Å. The hexagonal GaN nanowires are enclosed by six side (10-10) facets, shown in Fig. 1 (b). Figure 2 shows the cohesive energy of GaN nanowires as a function of diameter. As expected, the cohesive energy of GaN nanowire decreases as $1/D^2$ (D is the nanowire diameter) with increasing diameter.

The melting behavior of GaN nanowires is also investgated. We calculate the variation of the cohesive energy of GaN nanowires as the temperature is increased. The overall melting temperatures of GaN nanowires are much lower than that of bulk GaN and increase when the diameters of the nanowires are increased. These results are agreement with the trend for other nanowires.

To our knowledge, MD simulations for GaN nanowires using the empirical potential have not been reported so far. These theoretical calculations will provide considerable information about the possibility of GaN nanowires.

References

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[2] C. Y. Nam et al., Nano Lett., **6** (2006) 153.
[3] A. Bere and A. Serra, Phys. Rev. B, **65** (2002) 205323.

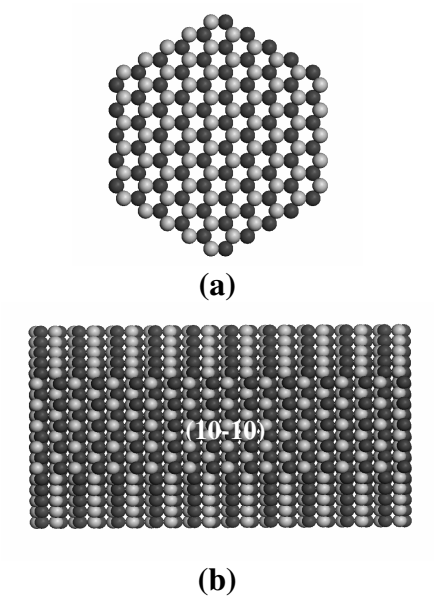

Figure 1. Optimized stuructre of GaN nanowire with the diameter of 28.67 Å. (a) Top view along the [0001] growth orientation. (b) Side view

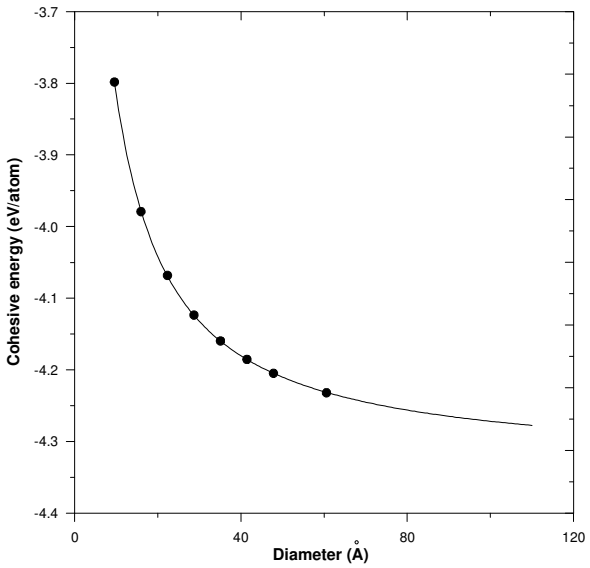

Figure 2. Cohesive energy of GaN nanowires as a function of diameter. The solid line is obtained by the least squares fit of data.