11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Stability of MgO nanowires

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Abstract – We present a theoretical investigation, based on first principles total energy calculations, on the structural properties of MgO nanowires. We explored nanowires in a number of cross section types and diameters. We find that MgO nanowires present little tendency to surface reconstruction, such that atoms on the wire surface sit in near-crystalline positions. We show that the stability of wires can be described using a simple phenomenological model that takes into account interactions between atoms and their first and second nearest neighbors. Additionally, we explored the trends in stiffness of those nanowires.

Oxide nanowires have attracted much attention over the last few years, for example because of potential applications as electronic components [1]. Magnesium oxide (MgO) emerged as a potential candidate in a number of applications, such as in the growth of core-shell ZnO/MgO nanowires with interesting luminescent properties [2,3]. MgO nanowires have been successfully grown using the Vapor-Liquid-Solid technique, resulting in long, vertically aligned, and self-organized structures [4].

Here, we explored the structural properties, stability, and stiffness of thin MgO nanowires based on *ab-initio* calculations. The calculations were performed using the density functional theory (DFT) in the local density approximation (LDA), using a plane wave basis set and pseudo-potentials. The Quantum Espresso package [5] was used to perform the calculations.

We explored nanowires in a number of cross section types and diameters, around 1 nm diameter and below, as described in Figure 1. We found that MgO nanowires present almost no surface reconstruction. Atomic displacements in-plane (perpendicular to the wire axis) are small and atoms on the wire surface sit near their ideal crystalline positions.

Using the results, we built a phenomenological model that describes the stability of the nanowires solely in terms of the interactions between atoms and their first and second neighbors. The model successfully describes all types of wires that have been studied. As a result, the stability of nanowires with larger cross sections could be predicted by this model.

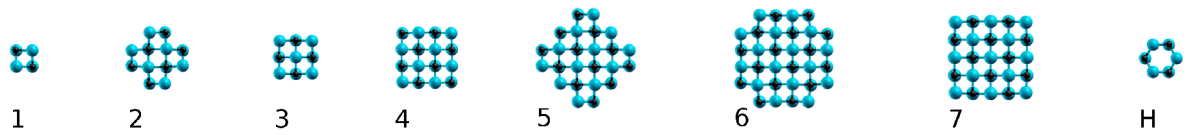

Figure 1: Geometries of the nanowires (cross sections perpendicular to the wire axis). Blue (black) balls represent magnesium (oxygen) atoms.

References

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