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A generalized thermophysical model for materials from molecular clusters to bulk crystals

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ABSTRACT

Evolution of properties of bulk materials from its molecular clusters has been a relatively unexplored topic. In this article, we present a generalized model for total thermal energy and heat capacity of solids by considering that a bulk solid is evolved from zero-dimensional molecular clusters through one-dimensional wires and two-dimensionalquantum sheets . The basic difference among these structures is shown to be the phonon density of states, which is continuous (unconfined) in a bulk solid, whereas it is confined in one, two, and three dimensions in QSs, QWs, and QDs, respectively. Considering a semi-empirically derived phonon density of states and the total unconfined and quantum confined dimensions in these structures, we arrived at a generalized equation. The generalized equation fits well to many experimental heat capacities including palladium and nickel nanoparticles, single-walled carbon nanotubes, and cadmium selenide quantum dots with high degree of accuracy ($R^2 > 0.99$). This close agreement between experiments and the generalized equation derived herewith provide promising directions to understand the evolution of bulk properties of materials.

1. Introduction

Materials discovery is at the heart of the human progress [1–6]; in the modern times, more materials are to be developed from renewable sources through low carbon processing to offset the carbon emission from material sourcing and processing [7–10]. Materials discovery is a laborious process through a multidisciplinary approach [11,12]; the understanding of increasingly complex material structures and the relationship with materials behavior brings the theoretical aspect in materials physics as the important roles to provide a conceptual paradigm for understanding the structure and properties of materials, and to sharpen the interpretation of experimental data [12,13]. The theory of materials has became a second impetus of materials physics, which has worked closely with experiments to interpret results and to investigate materials behavior under situations that cannot be examined directly by experiments [13]. The materials theory continued to play an important role in progressing materials physics, not only in terms of establishing mathematical models to explain the increasing complexity of materials [12,14] but also in terms of facilitating predictive data-driven materials research [13]. One of the unsolved issues in the materials discovery process is understanding the evolution of properties of materials from molecules to bulk solids, which has been a fascinating subject for physicists and chemists for a long time. Emergence of nanomaterials, which are midway between molecules and crystals, are enormously helpful in unravelling new properties [15,16]. Progress in processing materials from very low dimensionality such as zero-dimensional molecular clusters (*i.e.*, quantum dots, QDs) and the knowledge that their properties can be fundamentally different than a bulk solid provide opportunities to unravel the evolution of materials properties [15–19].

In this article, we track the evolution of thermophysical properties of semiconductors from its molecular clusters to bulk crystals. Semiconductors are chosen in this study because of the stable low-dimensional structures in them such as zero-dimensional quantum dots (QDs), one-dimensional quantum wires (QWs), two-dimensional quantum sheets (QSs) in addition to their bulk crystal (three dimensional) [17,20–22]. Typically, we examine the heat capacity of materials, which is one of the well-researched topics not only on the structure-property and processing-property relationship aspects of most of the known materials [23,24] but also using it as a tool to explain a variety of physical phenomena including lattice anharmonicity and lattice expansion [23,25–30]. The most frequently used [31] and widely applicable [32] heat capacity models that obeyed by many materials

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