Analysis of Transient Thermal Rectification using NEMD

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OVERVIEW

This study is focused on designing materials and systems of materials that lead to more energy efficient operation. In particular, the focus is on materials and systems that act as thermal rectifiers, which means materials and structures that transmit heat asymmetrically.

IMPORTANCE

We solved the non-linear heat equation and showed for a generic composite system of two materials the benefits of transient thermal rectification. Now, we want to demonstrate its importance using a real composite system. Good selection of materials is crucial because they must have promising applications and also must meet the conditions for having thermal rectification analyzed previously.

APPROACH

By using Nonequilibrium Molecular Dynamics Simulations (NEMD), we will analyze a system composed of two real materials to shows significantly higher levels of thermal rectification in transient state in comparison with values at steady state. We will compare results obtained using this methodology with those obtained by solving the non-linear heat transfer equation.

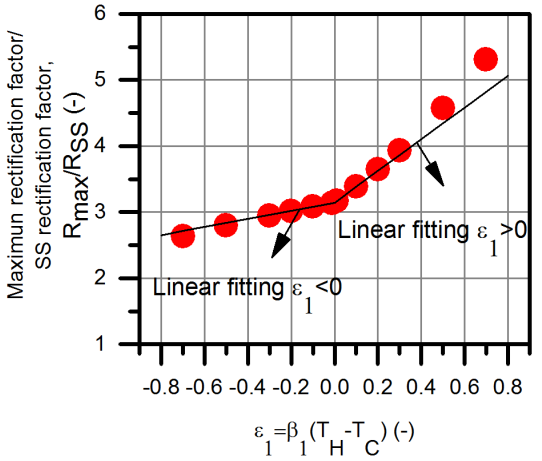

Fig. 1: Results of thermal rectification factor by solving non-linear Heat Transfer Equation.

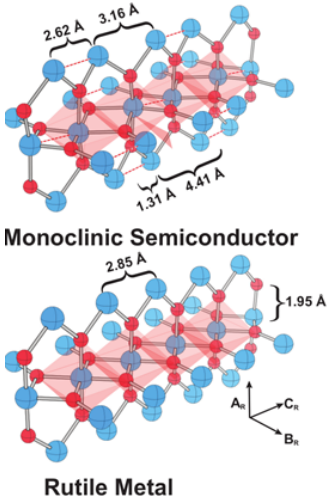

Fig. 2: Structure for potential material for study: Vanadium Dioxide (VO_2).

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