Drexel University
Department of Materials Science and Engineering

Investigation of Lattice Vibrations in Select $M_{n+1}AX_n$ Phases

PhD Dissertation Proposal

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July 11, 2011
10:00 AM
MEM Seminar Room
Curtis 162

Abstract

It is an interesting fact of physics that matter can never be completely motionless. Although objects that surround us may appear to be standing still, everything is made of atoms that are bonded together with interatomic forces and are constantly deviating form their equilibrium positions. Thus, all atoms that make up materials are consistently vibrating. When considering material properties, atomic vibrations come into play in a variety of ways. They play a major role in heat transport and other thermodynamic properties, and they can affect electronic transport as electron scatterers. They are also central to thermal expansion and high-temperature thermal stability, as the increased vibrations at high temperatures lead to larger interatomic distances and higher vacancy concentrations, among other phenomena.

Atomic vibrations tend to manifest differently in different types of materials. For this work, their role will be investigated for a group of materials known as MAX phases that exhibit a unique set of properties, combining some of the best attributes of ceramics and metals. As a class of materials with unprecedented property combinations, atomic motion is central to many different aspects and is especially important in considering their high-temperature damping and their thermal conductivity. Experimental and theoretical studies have suggested that certain MAX phases exhibit correlated atomic motion, which may be due to the strongly localized low-frequency modes where the atoms move in a synchronized way to avoid collision. The aim of this work is to further investigate these anharmonicity effects and explore the role of correlated atomic motion in select MAX phases. The effects of the chemistry, stoichiometry, and mass of the constituent atoms on the lattice dynamics will be examined. It will also be considered how the atomic motion, in turn, affects thermal transport properties, high-temperature stability, and damping. The time- and space-averaged thermal displacements, as well as the interatomic distance between atom pairs averaged over time, will be determined from *ab intio* calculations of the phonon density of states along with molecular dynamics simulations. These will be directly compared with experimental results from high-temperature neutron scattering, low-temperature Raman spectroscopy, and high-temperature x-ray diffraction.

Ultimately, the goal of this research is to fully characterize anharmonic atomic vibrations in MAX phases at low, ambient, and elevated temperatures through various theoretical and experimental techniques. In this proposal, the relevant background information, preliminary results, methodology, and research plan will be presented.