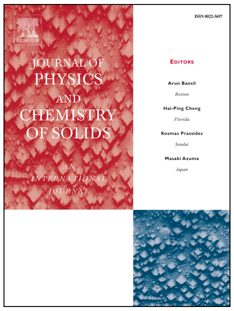

Calculation of the debye temperatures of hexagonal crystals from elastic constants

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Calculation of the Debye Temperatures of Hexagonal Crystals from Elastic Constants

Reed A. Howald

Abstract

Hexagonal crystals are less symmetric than cubic crystals, but the integrations to calculate debye temperatures from single crystal elastic constants are simpler and easier for hexagonal crystals. Houston's method actually works for hexagonal crystals in contrast to cubic crystals where it fails. The literature on these calculations for hexagonal crystals is reviewed and checked against modern computer calculations, and errors both small and substantial have been found in the use of Houston's method for hexagonal crystals in published papers. Examples of correct calculations of transverse, longitudinal, and overall debye temperatures are given for eleven different hexagonal crystals of interest, and for a number of arbitrary sets of elastic constants in the Wolcott tables. Mixing of longitudinal and transverse modes is a major problem for some cubic crystals, but appears to be less for known hexagonal crystals. The mixing of modes was examined for a particular case of C_{44} greater than C_{11} for one set of values covering hexagonal, tetragonal, and cubic symmetries. The one integration for any hexagonal crystal that can be performed analytically is also reviewed.

Introduction

It is important to know the thermodynamic properties of solids. Knowing the entropy of a pure solid at the temperatures and pressures of interest is probably the most difficult and complex problem in this area. Most of the tabulated entropy values for solids are based on measured heat capacities but measured values of C_p are usually available only at atmospheric pressure. The confinement required for higher pressures makes heat capacity measurements extremely difficult.

Fortunately thermodynamic variables are interdependent and one can often find an alternative way to get the result one wants. And while velocities of sound waves, and the single crystal elastic constants used to express them, are not really equilibrium properties of crystals they provide one of the best methods of getting heat capacities at low temperature and entropies of crystals at high pressure. The Wolcott tables[1] are one available method of going from single crystal elastic constants to debye remperatures for hexagonal crystals and a general overview of such methods is available in the Alers[2] paper.

Entropy for any material can be evaluated by an integration of C_p/T from 0 K to any temperature one desires. Because there is a temperature value in the denominator, it is especially important to somehow get really accurate heat capacity values at very low temperatures. While the debye theory has its limitations, it works well at the very low temperatures where it is needed for accurate entropies. The only other major contributions to heat capacities beyond the transverse and longitudinal vibrations are the higher energy vibrations, electronic heat capacity for metals and magnetic effects. Getting good debye temperatures for the transverse and longitudinal vibrations from elastic constants often gives