thermal vibration

The concepts of temperature and thermal equilibrium associated with crystal solids are based on individual atoms in the system possessing vibrational motion. The classical theory of thermal energy by atomic vibrations, though providing suitable explanations at elevated temperatures, has proved unsatisfactory at reduced or cryogenic temperatures. Quantum mechanics has subsequently provided theories based upon statistical probability that have provided possible mechanisms to explain some of the observed phenomena. A system of vibrating atoms in a crystal is highly complicated, and beyond the realm of any realisable theoretical method of analysis or calculations to verify spectral measurements from the total thermal energy of a crystalline substrate.

When a particle is bound to a crystal, the energy can only have discrete values as defined by the energy band structure. The quantum-mechanics of a one-dimensional simple harmonic oscillator gives permitted energies of (n+½)?? where ? is the angular frequency and n is the permitted energy integer. At a position of minimum energy (0K) the energy can never be zero, but has energy of ½??(zero-point energy) and as such will still provide crystal vibration.

As an atom can vibrate independently in three dimensions it is equivalent to three separate oscillators. The total thermal energy for N atoms will then be 3NkT, ignoring the ½?? term, the specific heat required to change the temperature by one degree will then be 3Nk where the specific heat of a solid for a given number of atoms is independent of temperature if N is the Avogadro number (6.02x1023). A detailed calculation of this form would require a knowledge of the number of atoms vibrating with frequencies ?1 ... ?n, which would depend on the density of states, and integration over the whole range of atomic vibrational frequencies would be required.

The thermal vibrations in a solid produce atomic displacements, which in a three dimensional lattice can be resolved into different states of polarization such that vibrations parallel to the wave vector are longitudinal waves and the two directions at right angles to the wave vector are transverse waves. As the rules of quantum mechanics apply to all the different atomic vibrations in the crystal, the lattice pulsates as a complete assembly in discrete energy steps of ??(phonons). The phonon is related to both the frequency of vibration and the temperature. If the temperature is raised, the amplitude of atomic vibration increases, and in quantum terms this is considered as an increase in the number of phonons in the system.

The concept of the phonon is therefore considered as the quantum of lattice vibrational energy onto which is superimposed a complex pattern of standing and/or travelling waves that represent changes in temperature. If the crystal is at a uniform temperature the standing wave concept is adequate as the phonon vibrations are uniformly distributed. http://www.reading.ac.uk/ir-absorptiontheory-thermalvibrations.aspx

The Lindemann relationship between the Debye characteristic temperature and the melting point may also be obtained from a consideration of the temperature variation of thermal diffuse x-ray scattering. The amplitude of thermal vibrations of the atoms in cubic crystals can be expressed in terms of the distance between neighbouring atomic positions and the melting point. This leads to a correlation of the relative increases of disorder on melting of body-centred cubic and face-centred cubic crystals with the thermal behaviour of the elastic constants, electrical resistance, atomic diffusion, specific heat, thermal expansion and thermal conductivity. A `law of corresponding states' may be said to exist where, at corresponding temperatures, the amplitudes of atomic vibration are the same fraction of the distance between neighbouring atomic positions in the solid. The Debye temperature factor is found to be inversely proportional to the melting point for cubic structures. http://iopscience.iop.org/article/10.1088/0370-1301/68/11/321/meta

See Also

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07 - Resonance Co-vibration or Sympathy of Tones
atomic vibration
attractive vibration
Chladni Plate Vibrations

Co-vibration
Compound Vibrations
electric vibration
Electricity from Vibration
ELECTRICITY FROM VIBRATION - Snell
ENERGY FROM VIBRATION - CONDENSATION OF MATTER THROUGH VIBRATORY INDUCTION
Equation by vibration
etheric vibration
Etheric Vibration. - The Key Force
Figure 3.11 Thermal Polarization
first and second order of atomic vibration
frequencies of consciousness vibrations
Healing Vibration, Personal
HEAT FROM VIBRATION
Inaudible Vibration
INAUDIBLE VIBRATIONS
INDUCTED VIBRATIONAL RANGES
interatomic vibration
intersympathetic vibration
Isothermal Process
Law of Corporeal Vibrations
Law of Harmonic Vibrations
Law of Sympathetic Vibration
Laws of Vibration
MASS VIBRATIONS
Modes of Vibration
Modes of Vibration - Annotated
molecular vibration
MOLECULAR VIBRATIONAL RANGE
negative vibration
nodal vibration
Orders of Vibration
Part 08 - What Vibration Is. - Part 1
Part 09 - What Vibration Is. - Part 2
Part 13 - Rotation from Vibration and Oscillation
Part 26 - Science of Sound Vibration Acoustics and Music
PHYSICAL VIBRATIONS
Planetary Vibration
positive vibration
Pressure produced by Vibration
PRESSURES PRODUCED BY VIBRATION
progressive vibration
propulsive vibration
propulsive vibrations
receptive vibration
REVOLVING SPHERE ROTATED BY VIBRATIONS
ROTATION FROM VIBRATION
Rotational-vibrational coupling
Rovibrational coupling
Sound and Vibration Definitions
spiritual order of vibration
sympathetic etheric vibration