Phonons in BCC Zr AT Various Temperatures

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ABSTRACT

In body-centered cubic (bcc) Zr, as temperature increases, certain low-energy phonons become unstable and are overdamped, which are precursors to martensitic phase transitions. Specifically, a longitudinal phonon mode drives the transition to the transverse phonon mode near polarization is responsible for the transition to the low- temperature hexagonal close-packed (hcp) phase. These low-frequency, damped phonon fluctuations are precursors to the low-symmetry phases within the bcc structure.

Keywords: BCC, Zr, temperatures, phase, phonon, hcp

INTRODUCTION

Temperature effects on phonons in bcc Zr Low-energy, overdamped phonons: At various temperatures within the bcc phase, certain specific phonon modes are found to have very low energy and are overdamped. Phase transition precursors: The longitudinal phonon mode's large displacement is related to the transition towards the phase. The transverse phonon mode with polarization is linked to the shift of bcc planes into the stacking sequence of the hcp phase. Softening: As the temperature approaches the phase transition, the phonons soften further but do not completely vanish, indicating a dynamic precursor to this transition. Stabilization: The vibrational entropy, driven by these low-energy phonons, is a significant factor in stabilizing the high-temperature bcc phase. Computational studies: First-principles and molecular dynamics simulations confirm these findings by calculating the phonon dispersion at various temperatures and observing phonon renormalization, notes ScienceDirect.com and arXiv. [1,2,3]

Zirconium (Zr) exhibits different properties and crystal structures at various temperatures, including a solid-state phase transformation and high melting and boiling points.

Behavior and Properties at Different Temperature Ranges Low to Moderate Temperatures (below 863 °C): Zirconium exists in the stable phase. It maintains excellent corrosion resistance due to a stable, passive oxide film that forms on its surface in air. At very low temperatures (below 35 K), some zirconium-niobium alloys become superconducting. Elevated Temperatures (above 863 °C): The crystal structure changes to the phase. This phase is less resistant to certain chemical attacks, notably rapid oxidation by high-temperature steam in a loss-of-coolant accident scenario in nuclear reactors, which produces hydrogen gas and has safety implications. Very High Temperatures (above 1855 °C):

Zirconium is in its liquid state. Extreme Temperatures (in compounds): Zirconium dioxide or zirconia, is a highly thermostable ceramic with a very high melting point of around 2715 °C (2988 K). It is used in refractory materials and as a thermal barrier coating in jet engines due to its mechanical strength and stability at extreme heat. Zirconium tungstate is an unusual compound that shrinks when heated (negative thermal expansion) up to 700 °C.

The behavior of phonons changes with temperature: at low temperatures, phonons are quantized and follow quantum mechanics, while at high temperatures, they behave more classically and exhibit anharmonicity, leading to effects like thermal broadening and softening (phonons shifting to lower energies). At very high temperatures, interactions between phonons become more complex, and their properties are often affected by other factors like magnetic transitions.

Low temperatures

Phonons are the quantized, low-energy vibrations of atoms in a crystal lattice.

Their behavior is predictable and can be accurately modeled by quantum mechanics. The Debye model is often used to describe phonons at low temperatures.

High temperatures

At higher temperatures, the classical, Dulong-Petit law begins to apply, which states that the specific heat is constant.[4,5,6]

Anharmonicity becomes more significant, leading to phonon-phonon interactions that cause them to behave in more complex ways.

Phonon softening: Phonon energies decrease (soften) as temperature increases due to thermal expansion.

Thermal broadening: Phonon peaks in the density of states broaden, especially for high-energy modes.

In some cases, such as materials with magnetic properties, magnetic transitions can significantly influence phonon behavior, especially at high temperatures.

Interactions with other excitations: Phonons can interact with other particles, like electrons, which can affect their properties and temperature dependence.

DISCUSSION

Phonons in a body-centered cubic (bcc) structure are quantized lattice vibrations that can be visualized as waves traveling through the crystal. Their behavior is described by phonon dispersion curves, which are often studied for their relationship to material properties and phase transitions. Specific features in bcc phonon dispersion, such as a "valley" of low-energy, strongly damped phonons, are characteristic and are linked to the displacements needed for phase transformations to more stable close-packed structures like hexagonal close-packed (hcp).

Key characteristics of phonons in bcc

Phonon dispersion curves: These plots show the relationship between the phonon frequency and its wave vector, providing insight into the lattice dynamics of the bcc structure.

Anharmonicity: Phonons in bcc metals are often strongly anharmonic, meaning their vibrations are not perfectly harmonic (like ideal springs). This is especially true for low-energy modes.

Relationship to phase transitions:

A common feature in many bcc metals is a band of low-energy, strongly damped phonons along specific directions in the Brillouin zone, such as.

The atomic displacements associated with these low-energy phonons are the same as those required for phase transformations to lower-energy structures, such as the ω or hcp phases, under certain conditions like pressure or temperature changes.

The stability of the bcc structure is sometimes explained by the contribution of these low-energy modes to the lattice entropy.[7,8,9]

Phonon scattering: Some bcc materials, like tungsten and molybdenum, exhibit weak phonon-phonon scattering, particularly along certain paths in the Brillouin zone. This is related to the small frequency differences between specific acoustic branches.

Electron-phonon coupling: Phonons play a crucial role in phenomena like superconductivity, where they mediate the interaction between electrons. For bcc metals, theoretical calculations are used to determine the strength of this electron- phonon coupling.

The phonon density of states (DOS) gives insight into interatomic forces and provides the vibrational entropy, making it a key thermodynamic function for understanding alloy phase transformations. Nuclear resonant inelastic x-ray scattering and inelastic neutron scattering were used to measure the chemical dependence of the DOS of bcc Fe–Co alloys. For the equiatomic alloy, the A2→B2 (chemically disordered→chemically ordered) phase transformation caused measurable changes in the phonon spectrum.

The measured change in vibrational entropy upon ordering was −0.02±0.02 k_B/atom, suggesting that vibrational entropy results in a reduction in the order–disorder transition temperature by 60±60 K. The Connolly–Williams cluster inversion method was used to obtain interaction DOS (IDOS) curves that show how point and pair variables altered the phonon DOS of disordered bcc Fe–Co alloys. These IDOS curves accurately captured the change in the phonon DOS and vibrational entropy of the B2 ordering transition.

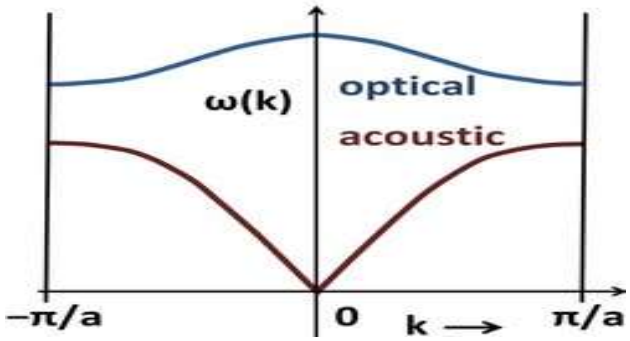
RESULTS

A phonon is a quasiparticle, collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids. In the context of optically trapped objects, the quantized vibration mode can be defined as phonons as long as the modal wavelength of the oscillation is smaller than the size of the object. A type of quasiparticle in physics,[1] a phonon is an excited state in the quantum mechanical quantization of the modes of

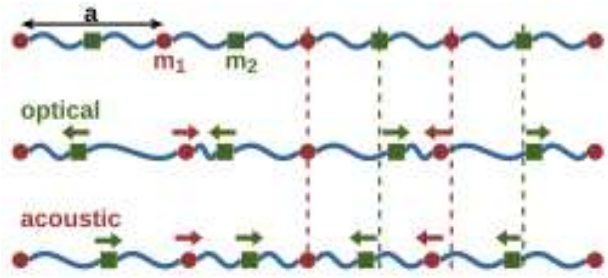
vibrations for elastic structures of interacting particles. Phonons can be thought of as quantized sound waves, similar to photons as quantized light waves.[2]

The study of phonons is an important part of condensed matter physics. They play a major role in many of the physical properties of condensed matter systems, such as thermal conductivity and electrical conductivity, as well as in models of neutron scattering and related effects.

The concept of phonons was introduced in 1930 by Soviet physicist Igor Tamm. The name phonon was suggested by Yakov Frenkel.[3] It comes from the Greek word φωνή (phonē), which translates to sound or voice, because long-wavelength phonons give rise to sound. The name emphasizes the analogy to the word photon, in that phonons represent wave-particle duality for sound waves in the same way that photons represent wave-particle duality for light waves. Solids with more than one atom in the smallest unit cell exhibit both acoustic and optical phonons. A phonon is the quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency.[4] In classical mechanics this designates a normal mode of vibration. Normal modes are important because any arbitrary lattice vibration can be considered to be a superposition of these elementary vibration modes (cf. Fourier analysis). While normal modes are wave-like phenomena in classical mechanics, phonons have particle-like properties too, in a way related to the wave–particle duality of quantum mechanics.[10,11,12]



Dispersion curves in linear diatomic chain



Optical and acoustic vibrations in a linear diatomic chain.

Acoustic phonons are coherent movements of atoms of the lattice out of their equilibrium positions. If the displacement is in the direction of propagation, then in some areas the atoms will be closer, in others farther apart, as in a sound wave in air (hence the name acoustic). Displacement perpendicular to the propagation direction is comparable to waves on a string. If the wavelength of acoustic phonons goes to infinity, this corresponds to a simple displacement of the whole crystal, and this costs zero deformation energy. Acoustic phonons exhibit a linear relationship between frequency and phonon wave-vector for long wavelengths. The frequencies of acoustic phonons tend to zero with longer wavelength. Longitudinal and transverse acoustic phonons are often abbreviated as LA and TA phonons, respectively.

Optical phonons are out-of-phase movements of the atoms in the lattice, one atom moving to the left, and its neighbor to the right. This occurs if the lattice basis consists of two or more atoms. They are called optical because in ionic crystals, such as sodium chloride, fluctuations in displacement create an electrical polarization that couples to the electromagnetic field.[2] Hence, they can be excited by infrared radiation: the electric field of the light will move every positive sodium ion in the direction of the field, and every negative chloride ion in the other direction, causing the crystal to vibrate.[13,14]

Optical phonons have a non-zero frequency at the Brillouin zone center and show no dispersion near that long wavelength limit. This is because they correspond to a mode of vibration where positive and negative ions at adjacent lattice sites swing against each other, creating a time-varying electrical dipole moment. Optical phonons that interact in this way with light are called infrared active. Optical phonons that are Raman active can also interact indirectly with light, through Raman scattering. Optical phonons are often abbreviated as LO and TO phonons, for the longitudinal and transverse modes respectively; the splitting between LO and TO frequencies is often described accurately by the Lyddane–Sachs–Teller relation.

When measuring optical phonon energy experimentally, optical phonon frequencies are sometimes given in spectroscopic wavenumber notation, where the symbol ω

The description of the atomic displacements by the harmonic approximation assumes that the force on an atom is a function of its displacement with respect to neighboring atoms, i.e. Hooke's law holds.[5] Higher order anharmonicity terms can be accounted by using perturbative methods.[6]

CONCLUSION

Phonons can be labeled by the manner in which the vibrations occur. If the vibration occurs lengthwise in the direction of the wave and involves contraction and relaxation of the lattice, the phonon is called a "longitudinal phonon". Alternatively, the atoms may vibrate side-to-side, perpendicular to wave propagation direction; this is known as a "transverse phonon". In general, transverse vibrations tend to have smaller frequencies than longitudinal vibrations.[5]

The wavelength of the vibration also lends itself to a second label. "Acoustic" branch phonons have a wavelength of vibration that is much bigger than the atomic separation so that the wave travels in the same manner as a sound wave; "optical" phonons can be excited by optical radiation in the infrared wavelength or longer.[5] Phonons take on both labels such that transverse acoustic and optical phonons are denoted TA and TO, respectively; likewise, longitudinal acoustic and optical phonons are denoted LA and LO.[16,17,18]

The type of surface phonon can be characterized by its dispersion in relation to the bulk phonon modes of the crystal. Surface phonon mode branches may occur in specific parts of the SBZ or encompass it entirely across.[1] These modes can show up both in the bulk phonon dispersion bands as what is known as a resonance or outside these bands as a pure surface phonon mode.[4] Thus surface phonons can be purely surface existing vibrations, or simply the expression of bulk vibrations in the presence of a surface, known as a surface-excess property.[3]

A particular mode, the Rayleigh phonon mode, exists across the entire BZ and is known by special characteristics, including a linear frequency versus wave number relation near the SBZ center.[19,20]

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