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Isotopic disorder effect in the infrared reflection spectra of $^{6}Li_x{}^{7}Li_{1-x}YF_4$ single crystals

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Abstract

Polarized infrared reflection spectra of $LiYF_4$ single crystals with different compositions of ^{7}Li and ^{6}Li isotopes were measured and analysed using the model of independent oscillators. Lattice dynamics calculations were performed. It was found that, for some modes, the contribution of the isotopic disorder to the damping constant is comparable to the anharmonic width. Results of simulations agree qualitatively with the experimental data. Possible reasons for the remaining discrepancies are discussed.

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1. Introduction

Isotopic disorder is the simplest type of disorder in crystal lattices. It contributes only to a random variation of atomic masses, while interactions between atoms remain unaltered. In some cases the isotopic disorder affects physical properties of materials significantly. One of the recently discovered isotope effects that is important for modern and future microelectronics is a large increment in the thermal conductivity of Si crystals after isotopic purification (about eight times at $T = 26$ K, and ∼10% at room temperature) [1]. Though isotope effects in solids have been studied for a long time, the recent interest in them is motivated by novel applications and the improvement in experimental facilities. Comprehensive reviews on isotope effects in solids and on their applications can be found, for example, in Refs. [2,3].

Different isotope effects have been observed in optical spectra of crystals, in particular in infrared spectra of bulk NaCl and LiF crystals [4–6], infrared spectra of donor and acceptor impurities in Si [7,8], Raman spectra of bulk semiconductor crystals [9], in optical spectra of transition metal [10] and rare-earth [11,12] ions embedded in crystal lattices.

Here we report results of measurements and simulations of isotope effects in the infrared (IR) reflection spectra of $LiYF_4$ single crystals due to mass disorder in the lithium sublattices. The crystal $LiYF_4$ is widely used as a host matrix for rare-earth ions in solid-state lasers [13]. It has been shown that pseudo-splittings of optical lines in rare-earth-doped $LiYF_4$ crystals due to isotopic disorder in Li sublattices may be as much as 0.03 cm^{-1} [12,14]. In this context, our study is important for the purposes of solid-state quantum electronics. We should emphasize that the IR spectra of $LiYF_4$ were studied comprehensively in Ref. [15], however the isotope effects have not been addressed.

2. Experimental

The $LiYF_4$ crystal belongs to the space group C_{4h}^6 with two formula units in the unit cell. Lattice vibrations at the Brillouin zone centre are classified by irreducible representations of the C_{4h} factor group. There are 12 IR active modes, namely four

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