Spectra of Optical Magnons in Bulk Iron

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We present the results of the numerical studies of the spectra of optical magnons in bcc Fe at room conditions (𝑇 ≈ 298 K and 𝑃 ≈ 1 bar). Recently, we modelled spectra of phonons and magnons in bcc-iron at these conditions by dynamic structure factors (DSF) calculations and with the aid of Chamati potential [1-3]. It has been shown that use of this potential developed within the embedded-atom method gives the best agreement between our calculated in DSF procedure and experimental phonon and magnon spectra. The exchange parameter has been evaluated on the base of the calculated magnon spectra in the long wavelength limit. Then, the spectrum of optical magnons has been obtained numerically with the aid of the exchange parameter determined. We expect strong phonon-magnon interaction owing to peculiarities in their spectra. Our findings provide valuable insights for theorists, experimentalists and developers of new magnetic and phononic materials and devices.

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[3] E. Angelova, H. Chamati, Spectra of elementary excitations in bulk iron, ACS Omega (2025) (in print).