

Phonons and magnons in high-magnetocrystalline-anisotropy Fe–Co random alloy — from first principles density functional theory calculations to atomistic simulations

Wojciech Marciniak,^{1,2} Joanna Marciniak,^{1,3} Martin Ošmera,¹ José Ángel Castellanos-Reyes,¹ Mirosław Werwiński,³ and Ján Ruzs¹

¹*Department of Physics and Astronomy,
Uppsala University, P.O. Box 516, 751 20 Uppsala, Sweden*

²*Institute of Physics, Poznań University of Technology,
Piotrowo 3, 60-965 Poznań, Poland*

³*Institute of Molecular Physics, Polish Academy of Sciences,
M. Smoluchowskiego 17, 60-179 Poznań, Poland*

Since the discovery of high-magnetocrystalline-anisotropy region by Burkert *et al.* in 2004 [1], tetragonally strained Fe–Co random alloy has been thoroughly investigated. Recently, we reported a second giant-MAE region for the same alloy under uniaxial compression [2].

Static picture is, however, not enough for technological applications. In finite-temperature contexts, it is essential to explore cohesive dynamical effects such as phonons and magnons. Notably, the recent direct observation of magnons via (scanning) transmission electron microscopy [(S)TEM] [3] complements earlier detections of phonons [4], pointing towards (S)TEM as a viable tool for examining both spin magnetic moment and atomic dynamics.

In this context, we have developed a method that allows for an investigation of wave-vector- and frequency-resolved phonon mode dynamics in solids [5]. This approach has the potential to be expanded to encompass spin and spin-lattice systems, aligning with the principles of atomistic spin(-lattice) dynamics – AS(L)D [6].

Here, we will present a broad spectroscopic picture of phonon and magnon dynamics in high-anisotropy permanent magnet — Fe–Co.

References:

- [1] T. Burkert, *et al.*, Phys. Rev. Lett. **93** (2004), 027203
- [2] W. Marciniak, *et al.*, arXiv preprint (2024), arXiv:2409.11388
- [3] D. Kepaptsoglou, J. Á. Castellanos-Reyes, *et al.*, Nature **644** 8075 (2025): 83-88.
- [4] O. L. Krivanek, *et al.*, Nature **514** 7521 (2014): 209-212.
- [5] W. Marciniak, *et al.*, Ultramicroscopy **282** (2026): 114320
- [6] J. Hellsvik, *et al.*, Phys. Rev. B **99** (2019), 104302

We acknowledge support from the Swedish Research Council (grant no. 2021-03848), the Olle Engkvist Foundation (grant no. 214-0331), and the Knut and Alice Wallenberg Foundation (grant no. 2022.0079). The simulations were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at NSC Centre, partially funded by the Swedish Research Council through grant agreement no. 2022-06725.