Biswanath Dutta

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- https://scholar.google.nl/citations?user=--QBfw0AAAAJ&hl=nl&oi=ao

Research topics:

- Modelling finite temperature effects (e.g., phase stability)
- Molecular dynamics (empirical potential & ab initio) simulation
- Magnetic refrigeration
- Waste energy harvesting
- High entropy alloys

Ab initio design of functional and structural materials

Research activities:

Correlation between chemistry, atomic disorder and magnetocaloric effect:

Magnetocaloric materials have received a lot of attention in recent years due to their functional applications, which include energy efficient, environment friendly magnetic cooling and waste energy harvesting. In the quest to achieve improved magnetocaloric properties, different design strategies have been adopted. Using ab initio calculations, we have studied the impact of chemical doping and atomic disorder on the magnetic and the structural properties of Mn-excess NiMn-based Heusler alloys.

Based on our calculations, we identify Co and Fe as the most promising elements to improve magnetic properties of NiMn-based magnetocaloric materials. Our calculations reveal an antiferromagnetic to ferromagnetic transition above a critical amount of Co or Fe doping in the austenite phase of Mn-excess Ni-Mn-Al [1]. The martensite phase, however, remains antiferromagnetic, which explains the experimentally observed metamagnetic transition in these alloys. The obtained magnetic properties are explained on the basis of magnetic exchange interactions.

Our calculations also reveal a remarkable impact of atomic configuration on the structural and magnetic properties [2]. We find a delicate interplay of magnetic and chemical orders and the tetragonal distortion during the martensitic transformation. Based on these findings, we qualitatively explain the experimentally observed changes in the magnetocaloric properties after different annealing times.

Abnormal magnetic properties of FeNiCoMnCu high entropy alloy:

High entropy alloys are systems with multiple principal elements and have attracted attention due to their excellent mechanical, physical and chemical properties. In contrast, magnetic properties of these alloys remains uncharted. We investigate the effect of non-magnetic Cu on the magnetic properties of FeNiCoMn alloy (Z. Rao, **B. Dutta** et al., *in preparation*). Our study reveals an anomalous increase in Curie temperature and magnetization due to Cu addition. The abnormal trends are explained on the basis cumulative effect of volume and composition changes.

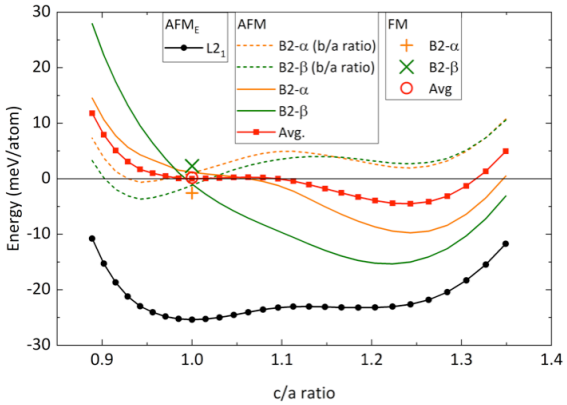

Figure 1: Change in energy as a function of c/a-ratio for the different atomic configurations studied for Ni-Co-Mn-Al [2]

Other activities

[A] Invited talk at Linköping University, Sweden
[B] Acted as peer-reviewer for 21 scientific articles (journals include Acta Materialia, Physical Review B, Intermetallics and Materials)

Key publications 2018:

[1] A. Waske, **B. Dutta** et al., Energy Technol. **6**, 1429 (2018).
[2] B. Weise, **B. Dutta** et al., Sci. Rep. 8:9147 (2018).
[3] P. Devi, S. Singh, **B. Dutta** et al., Phys. Rev. B **97**, 224102 (2018).
[4] Y. Ikeda, F. Körmann, **B. Dutta** et al., npj Comput. Mater. 4:7 (2018).