Construction of Landau-type free energy from experimental phase diagrams using reverse modeling

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Finding the form of a free energy that describes complex phases of a solid based on limited physical insight is often a difficult task. We develop an automated approach for constructing a Landau-type free energy from experimental phase diagrams, starting from a general form for the free energy with given number of order parameters. The approach combines random search with local optimization to minimize the difference between the calculated phase diagram with the targeted phase diagram. To illustrate the method, it is applied to the magnetic field-temperature phase diagram of Mn(taa), and the free energy that agrees well with the experimental phase diagram is found.

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