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A data driven approach to the prediction of phase diagrams

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PURPOSE OF THE ABSTRACT

The knowledge of the phase diagrams is crucial to understand materials and to design new ones with better properties. In this work, we addressed the prediction of phase diagrams and crystal structures using a data-driven approach. We used machine learning methods to predict the stable phases using a set of diagrams contained in the NIST database. First, we extracted the data on composition, temperature, and pressure from the vectorial images, then, we integrated the knowledge from the figure with additional information extracted from the attached text description. After this data process, we trained machine learning algorithms to predict the stable phases and the molecular formula of the stable compounds. In addition, we use trained additional models to predict the Bravais lattice, crystal type and the local atomic environments of the inorganic compounds contained ICSD database.

FIGURES

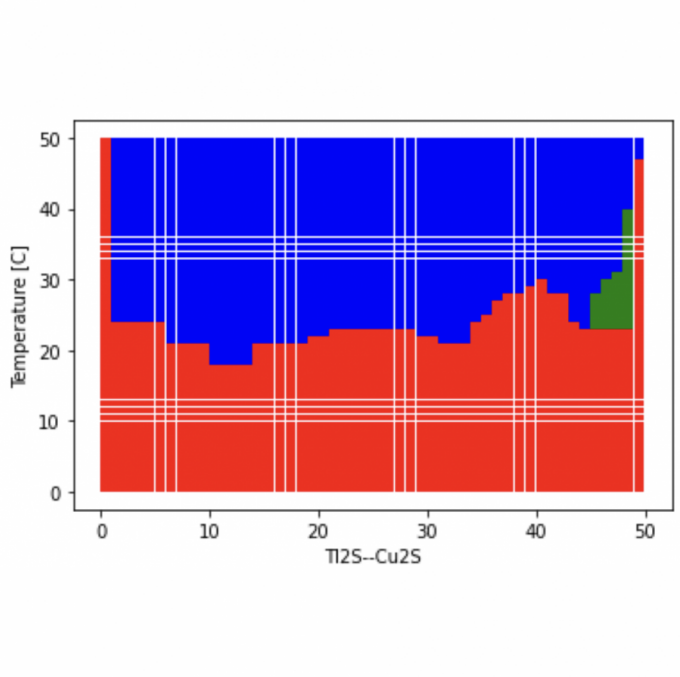

FIGURE 1

Predicted binary phase diagram.

The figure illustrate the phase diagram predicted for a two component system consisting of Tl2S/Cu2S at ambient pressure at different temperatures: the solid, liquid and mixed solid/liquid phases are colored in red, blue, and green.

FIGURE 2

KEYWORDS

artificial intelligence | crystal structures | machine lerning | phase diagrams

BIBLIOGRAPHY