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Spatiotemporal observation and modelling of temperature scan rate effects on the thermal hysteresis and the dynamics of interface propagation in a spin-crossover single crystal

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The direct observation by optical microscopy of the thermally-induced spin transition [1] and the subsequent low-spin high-spin interface propagation inside the thermal hysteresis is a fascinating problem. The kinetic aspects of the spin crossover (SCO) transition investigated under various scan rates was studied so far on powder sample which then average the kinetic effects of the thermal hysteresis. This problem is studied here on the robust spin-crossover single crystal $[\{Fe(NCSe)(py)_2\}_2(m\text{-}bpypz)]$ for which we followed the dynamics of the thermal hysteresis at several controlled temperature scan rates [2]. In addition to the expected shifts of the switching temperatures, sizable change in the velocity of the high-spin (HS) low-spin (LS) interface dynamics are observed for the first time. Theoretical developments based on a spatiotemporal description of the SCO phenomenon using reaction diffusion equations including the heat balance between the crystal and its immediate environment. We identified the competition between the heat transfer between the crystal and the thermal bath with the temperature scan rate kinetics as key parameter governing the interface velocity, at the origin of the kinetic features of the hysteresis. The experimental data are modelled using a reaction diffusion equation allowing to fairly reproduce the essential features of the spatiotemporal properties of the spin transition.

References

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