A Density of States-Based Approach for Thermally-Induced Aggregation Kinetics

L. F. Trugilho[1], S. Auer[2], L. G. Rizzi[1]

[1] Departamento de Física, Universidade Federal de Viçosa (UFV), 36570-900, Viçosa, MG, Brazil
[2] School of Chemistry, University of Leeds, Leeds LS2 9JT, Leeds, UK

Thermally-induced aggregation kinetics in finite systems with interacting particles is usually described by approaches which assume that the shape of the aggregates has a definite form, e.g., spherical, cylindrical, cubic. However, as in the case of aggregating particles with weak anisotropic interactions, that kind of assumption is unlikely to lead to reasonable approximations. Alternatively, we consider the density of states of the system to establish an approach that characterizes phase transformation rates in terms of shape-independent thermostatistical quantities which can be obtained directly from flat-histogram and statistical temperature algorithms. By performing simulations of an Ising-like model with anisotropically interacting particles at temperatures close to its first-order aggregation transition, we demonstrate that such approach can be used to describe thermally induced phase transformation kinetics in finite systems [1]. A quantitative comparison between the numerically obtained forward and reverse rates to approximated temperature-dependent expressions [2,3] is used to validate our procedure as a general shape-free and model-independent method.

The authors acknowledge the funding support received from CAPES (PDSE Scholarship), FAPEMIG (Doctorate Scholarship and support for attending the event), and CNPq (Grant N°312999/2021-6).

References

[1] L. F. Trugilho, S. Auer, L. G. Rizzi. A density of states-based approach to determine temperature-dependent aggregation rates. J. Chem. Phys. **161** (2024) 051101.

[2] L. G. Rizzi. Kinetics of first order phase transitions from microcanonical thermostatistics. J. Stat. Mech. **2020** (2020) 083204.

[3] L. F. Trugilho, L. G. Rizzi. Shape-free theory for the self-assembly kinetics in macromolecular systems. Europhys. Lett. (EPL) **137** (2022) 57001.

Type

ORAL