Poster Presentation

MS066.P04

Single-crystal-to-single-crystal phase transition by thermosalient effect in isomorphous schiff base

Ramesh Devarapalli[1], Chun-Teh Chen[2], Gang Seob Jung[2], Rama Krishna Gamidi[1], Sourabh Kadambi[3], Upadrasta Ramamurty[3], Markus J. Buehler[2], C Malla Reddy[1]

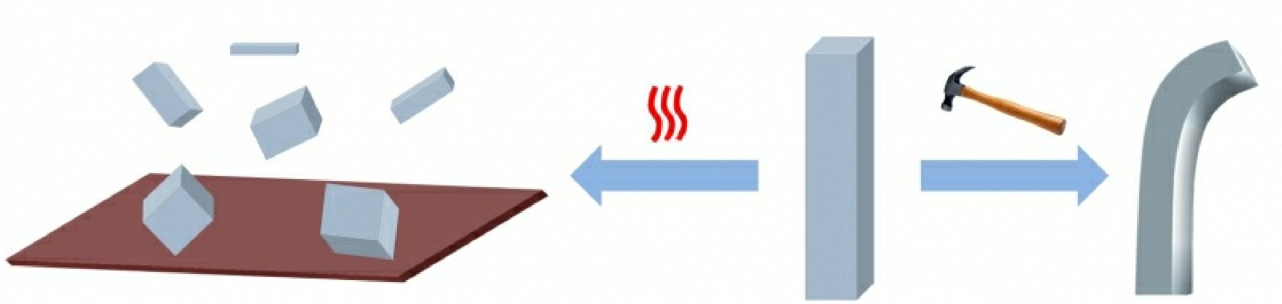
[1]*Department Of Chemical Sciences, IISER Kolkata, Mohanpur Campus, Mohanpur, India,* [2]*Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States,* [3]*Department of Materials Engineering, Indian Institute of Science, Bangalore, Bangalore, India*

E-mail: rameshpolvrm@gmail.com

Materials that respond to external stimuli like heat, light, and pressure are of immense importance in the conversion of respective energy to mechanical work. Such mechanically responsive materials are candidates for future dynamically active elements like artificial muscles, actuators, heat-responsive materials for electronics, sensors, and others. Single crystalline materials may be utilized fully in the development of technologically valuable actuators because of their highly ordered structures and ability of fast energy transport. However, the relationship between the changes in the crystal mechanical properties and crystal structure during a phase transition has remained relatively unexplored. In this study, a single-crystal-to-single-crystal phase transformation by heat as an external stimulus for two plastically bendable (under mechanical stress) isomorphous Schiff bases is studied by both experiments and molecular modeling simulations. Upon heating, the compounds viz. o-vanilidene-p-chloroaniline and o-vanilidene-p-bromoaniline were irreversibly converted to new polymorphs; interestingly these are also isomorphous as revealed by their cell parameters. The thermosalient effect of these two compounds was fully studied with the help of variable temperature single crystal X-ray structure determination, thermal analysis and with variable temperature powder X-ray diffraction data. The plastically bendable parent crystals convert to brittle polymorphs after phase transition. The plasticity and hardness of polymorphs were quantified with the nanoindentation technique. The reasons for such gratuitous mechanical properties were deeply investigated.

[1] Naumov, P. et al. (2013) Angew. Chem. Int. Ed. 52, 9990–9995.
[2] Ghosh, S. & Reddy, C. M. (2012) Angew. Chem. Int. Ed. 51, 10319–10323.
[3] Sahoo, S. C. et al. (2013) J. Am. Chem. Soc. 135, 13843−13850.

Depiction of jumping (left side) of single crystal on heating and plastic bending (right side) under mechanical stress.



Keywords: thermosalient phenomenon, phase transition, mechanical properties