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Periodic structure optimization via local heat pulse-quench cycles employing the GULP code ARNULF MÖBIUS, Institute for Theoretical Solid State Physics, IFW, Dresden, Germany, J. CHRISTIAN SCHÖN, Max Planck Institute for Solid State Research, Stuttgart, Germany — We present an optimization algorithm for problems with many continuous degrees of freedom and a huge number of local minima. It is based on the thermal cycling approach, originally developed for combinatorial optimization tasks [1]. The main idea is to cyclically disturb a few randomly chosen degrees of freedom of the current best local minimum and to quench this state by a highly efficient local search code. As the optimization proceeds, the amplitude of the disturbance slowly decreases. This approach is applied to a lattice structure prediction problem. We use the general utility lattice program (GULP) by J.D. Gale and co-workers [2] for local search. As test, the hypothetical periodic $Mg_{10}Al_4Ge_2Si_8O_{36}$ compound is studied, where both the cell parameters and the atom positions are free to vary. The results demonstrate that the proposed procedure is robust and far more efficient than the previous approaches to this problem by means of multi-start local search, simulated annealing, and evolutionary algorithms in Ref. 3.

[1] A. Möbius et al., Phys. Rev. Lett. 79 (1997) 4297.
[2] J.D. Gale and A.L Rohl, Mol. Simul. 29 (2003) 291.
[3] A.R. Oganov et al., in "Modern Methods of Crystal Structure Prediction," ed. A.R. Organov, (Wiley, 2011), p. 223.

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