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Calculation of formation energies of intrinsic point defects in In_3La JOHN P. BEVINGTON, Washington State University, Pullman, WA, GARY S. COLLINS, Washington State University, Pullman WA — We use *perturbed angular correlation of gamma rays*, or PAC, to measure jump frequencies of ^{111}In/Cd probe atoms in In_3La and related phases (see Phys. Rev. Lett. 92, 225019 (2004)). To interpret the jump frequencies, first principles calculations were used to determine energies of intrinsic vacancy and antisite atom defects. In_3La has the $L1_2$ structure in which four possible combinations of vacancies and antisite atoms can be thermally activated that maintain the homogeneity of the phase. Formation energies of the defect combinations were calculated using the electronic structure code WIEN2k that is based on density functional theory. Partial formation energies were found to be least for La_{In}, at 0.71 eV, and V_{In}, at 1.47 eV, with much greater energies for In_{La} and V_{La} defects. Formation energies per defect of the four defect combinations all had similar values, but the antisite pair, $La_{In} + In_{La}$, had the lowest value. *This work was supported by the NSF under grant DMR 05-04843 (Metals Program).*

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