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Density functional analysis of long range order T.R.S. PRASANNA, IIT Bombay — A density functional analysis of order-disorder transitions in alloys shows that ordering energy is stored in superlattice wavevectors. Thermal vibrations play a key role and lower the transition temperature, T_c, to the experimental value (741 K) from the mean-field value (933 K) in the Bragg-Williams model for beta brass, β-CuZn. An isotope effect with 4 K difference in T_c is predicted for $^{63}Cu^{64}Zn$ and $^{65}Cu^{68}Zn$ in a Modified Bragg-Williams model. The above conclusions are shown to be applicable in magnetic transitions as well. Theoretical analysis shows that thermal vibrations alter the exchange and total magnetic ordering energy. Every microscopic theory of magnetic and alloy phase transitions must satisfy the twin criteria that ordering energy is a) stored in superlattice wavevectors and b) a function of temperature due to thermal vibrations. An isotope effect is predicted to be a universal feature of alloy and magnetic phase transitions. The nuclear-nuclear energy term, E_{n-n}, converges without artificial parameters if zero point vibrations are included unlike the Ewald sum technique.

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