

Investigation about Structural and Optical Properties of Bulk and Thin Film of 1H-CaAlSi by Density Functional Method

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Abstract : Optical properties of bulk and thin film of 1H-CaAlSi for two directions (1,0,0) and (0,0,1) were studied. The calculations are carried out by Density Functional Theory (DFT) method using full potential. GGA approximation was used to calculate exchange-correlation energy. The calculations are performed by WIEN2k package. The results showed that the absorption edge is shifted backward 0.82eV in the thin film than the bulk for both directions. The static values of the real part of dielectric function for four cases were obtained. The static values of the refractive index for four cases are calculated too. The reflectivity graphs have shown an intensive difference between the reflectivity of the thin film and the bulk in the ultraviolet region.

Keywords : 1H-CaAlSi, absorption, bulk, optical, thin film

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