

MECHANISM FOR DICARBON DEFECT FORMATION IN AIAs AND GaAs

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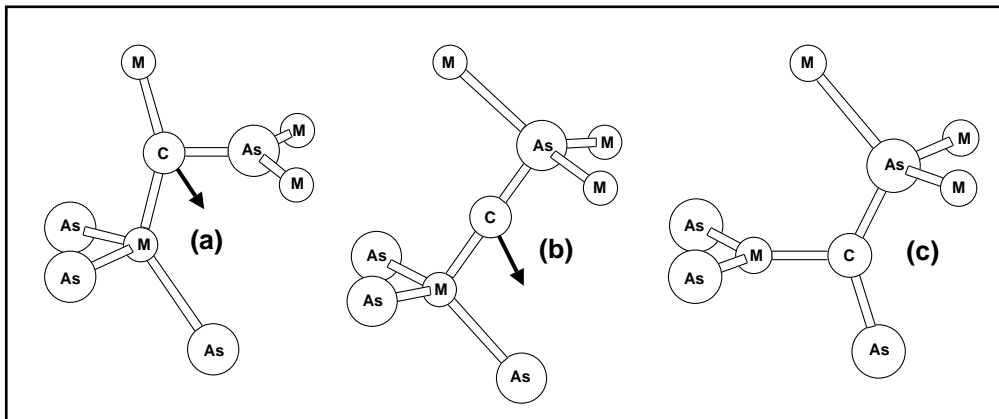
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There is a need to understand the degradation mechanism which results in the loss of substitutional C_{As} shallow acceptors in AIAs and GaAs containing high concentrations $\gtrsim 10^{20} \text{ cm}^{-3}$ of carbon. The activation energy for the migration of interstitial carbon atoms, C_i , in AIAs and GaAs is calculated using a local-density functional based method, AIMPRO, to be $\lesssim 1 \text{ eV}$. This model is consistent with a ‘kick-out’ mechanism being responsible for the observed loss of C_{As} , and formation of dicarbon defects. Three local minima separated by only a few tenths of an eV are encountered by a diffusing carbon atom along its path through the crystal. In order of decreasing energy these have $(C-As)_{As}$ split interstitial, bond-centred $M-C-As$, and $(C-M)_M$ split interstitial structures ($M = \text{Al, Ga}$). Interstitial dicarbon defects, $(C-C)_i$, or substitutional dicarbon defects, $(C-C)_{As}$, are produced depending on whether a C_i meets a $(C-M)_M$ split interstitial or a C_{As} . These possess Raman-active C-C vibrational modes near to that for a free dicarbon molecule, C_2 .



ABOVE: Diffusion mechanism for C_i in AIAs and GaAs: local minima are found at (a) $(C-As)_{As}$ split interstitial, (b) bond-centred C interstitial, and (c) $(C-M)_M$ split interstitial configurations along the migration path.

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