

Short Note



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Any electronic device cannot be build from any two different materials if their lattice thermal expansions are not in match. Most methods of experimental measurements and theoretical calculations to obtain this parameter in semiconductors are expensive and complicated. Some times they need large and costly computational programs. In my work, a new approach is achieved for calculating lattice thermal expansion for semiconductors.

Twenty four years ago, while I was working on my PhD research in England, I found an article about a model to calculate lattice thermal expansion in semiconductors. At that time, I felt that, the subject could be a key point for some interesting future research work in the named field.

In the last three years, the subject has become one of my selected interest works. The model was a simple empirical relation between the melting point, mean atomic bonding and lattice thermal expansion. It is applicable to compound groups having the same crystal structure and ionicity. The model is originally derived from group IV semiconductors and applied on III-V and II-VI compound semiconductors. In my work the model was used to calculate lattice thermal expansion for ternary group compounds of II-IV-V₂, I-III-VI₂ and I-IV₂-V₃ semiconductors. The relation was then, modified to include the fourth parameter of ionicity. The latter gives opportunity for the model to be applicable for calculating lattice thermal expansion for all compounds from the groups mentioned above. The compounds included (GaP, GaAs, GaSb, InP, InSb,) from III-V, (CdS, CdSe, ZnS, ZnSe,) from II-VI, (CuInS₂, CuInSe₂, CuGaS₂, CuGaSe₂,), from I-III-VI₂, (ZnSiP₂, ZnGeP₂, ZnSnP₂, CdGeP₂, CdSiP₂,) from II-IV-V₂ and (CuGe₂P₃, CuSi₂P₃) from I-VI₂-V₃. The results were published by *ELSEVIER Publication in Materials Research Bulletin 42 (2007) 319-323*. Later on, the model was extended to be applicable on two more complicated ternary groups of I₂-IV-VI₃ and I₃-V-VI₄ semiconductors. These compounds included (Cu₂GeS₃, Cu₂GeSe₃, Cu₂SiS₃...) from I₂-IV-VI₃ and (Cu₃PS₃, Cu₃PSe₃, Cu₃AsS₃, Cu₃AsSe₄...) from the group I₃-V-VI₄. This work was also accepted by the Journal mentioned above and it will appear in April 2007.

The work is in progress to extend the formula to be applicable on defect compound semiconductors of the group III₂-VI₃.

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