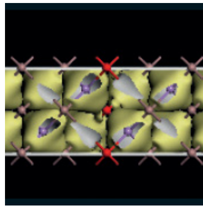


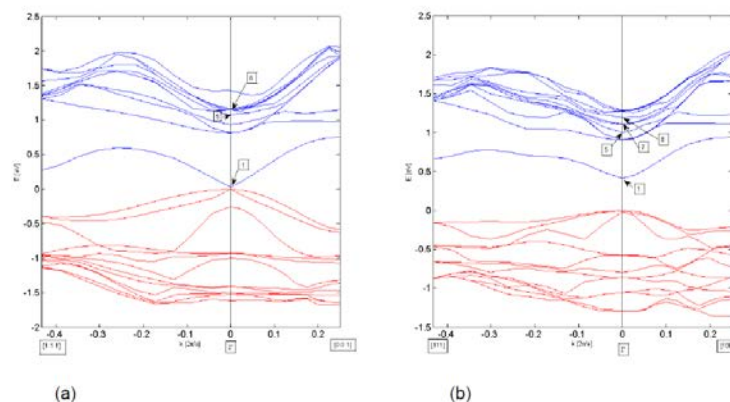
Electronic structure calculation of SiGeSn-C alloys – prospective direct gap materials

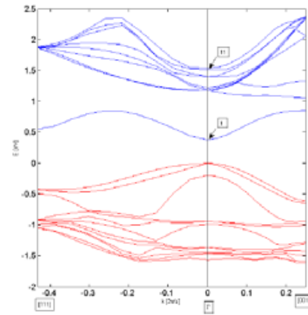
Z Ikonić[1] and D Buca[2]

[1]University of Leeds, UK, [2]Peter Grünberg Institute (PGI 9) and JARA-Fundamentals of Future Information Technologies, Germany

In the recent period large advances have been made in group-IV photonics (and also electronics), targeting the integration of group-IV alloy based (opto)electronic components on silicon substrate, with all the benefits coming from mature and cost-effective fabrication. This progress requires a reliable knowledge of the electronic band structure of CSiGeSn alloys, including their ternary and binary subsets. The directness of the band-gap is very important for optoelectronic devices – primarily lasers, as has been recently demonstrated [1], and also LEDs, photodetectors and modulators – very much improving the device performance. Along with the composition, the values of the direct and indirect gaps can be controlled by strain. The binary GeSn, and also the ternary SiGeSn alloys, which offer the direct band gap, have been studied in considerable detail, both experimentally and theoretically. An alternative way of achieving direct band gap in group-IV materials is in using dilute carbon alloys with other group IV's, which have been studied to some extent [2-6], with different predictions of the effects of C addition. This system is very different from the SiGeSn alloys, because C atom has a much larger electronegativity than the host, a very different lattice constant, the C-C bonds are stronger than C-Ge bonds, and such alloys normally have large density of C clusters and various defects which form trap states in the band gap, and do not lead to a high-quality direct gap material. However, recent successes in highly substitutional incorporation of C in very dilute Ge-C alloy, by using a suitable C source, have revived interest in this system.

Here we consider the band structure of Ge-C, and more generally SiGeSn-C alloys. The empirical pseudopotential method (EPM) is employed within the supercell approach (because the virtual crystal approximation is not applicable for C-containing alloys), with the formfunctions made so to reproduce the workfunctions of all the alloy constituents, along with their band structure. This was done by using constrained cubic spline interpolation between the fixed formfactors, the method which avoids artificial over/under-shoots between the fitting points. Calculations were made with 32-, 64- and 128-atom supercells, followed by unfolding procedure. Also calculated is the optical activity at the unfolded direct gap of various alloys (v.b.-c.b. optical matrix element, compared to that in Ge). Examples of the band structure are given in Fig.1(a,b,c). The sensitivity of direct and indirect band gaps to carbon content is also extracted for SiGe-C alloy system, Fig.1d (both decreasing with the C content, in contrast to what VCA would suggest, but gap at Γ doing so at a faster rate than indirect gaps at L and X). The Ge-C is predicted to become a direct gap material at ~0.2%C, still somewhat larger than contents which enable good quality substitutional alloy, however there are prospects of achieving direct gap in this system, with various possible applications.





Ge:Si	$dE_{\Gamma}/d(\%C)$	$dE_{X,L}/d(\%C)$
1:0	-0.59	-0.016
2:1	-1.15	-0.044
1:1	-1.41	-0.045
1:2	-1.65	-0.046
0:1	-1.91	-0.033

(c) (d)

Fig.1. Band structure of (a) C_1Ge_{63}, (b) C_1Ge_{127}, (c) $C_1Ge_{41}Si_{22}$, and (d) bandgaps sensitivity of different SiGe compositions to C content.

[1] S. Wirths, R. Geiger, N. von den Driesch, G. Mussler, T. Stoica, S. Mantl, Z. Ikonic, M. Luysberg, S. Chiussi, J. M. Hartmann, H. Sigg, J. Faist, D. Buca, D. Grutzmacher, "Lasing in direct bandgap GeSn alloy grown on Si (001)", Nature Photonics, 9, 88 (2015).

[2] R. Soref, “Direct-bandgap compositions of the CSiGeSn group-IV alloy,” Optical Materials Express, 4, 836 (2014).

[3] J. Kolodzey, P. R. Berger, B. A. Orner, D. Hits, F. Chen, A. Khan, X. Shao, M. M. Waite, S. Ismat Shah, C. P. Swann, K. M. Unruh, “Optical and electronic properties of SiGeC alloys grown on Si substrates”, J. Crystal Growth, 157, 386 (1995).

[4] M. Rezki, A. Tadjer, H. Abid, and H. Aourag, “Electronic structure of Si1-x-yCxGey”, Materials Science and Engineering B, 55, 157 (1998).

[5] T. Yamaha, K. Terasawa, H. Oda, M. Kurosawa, W. Takeuchi, N. Taoka, O. Nakatsuka, and S. Zaima, “Formation, crystalline structure, and optical properties of Ge1-x-ySnxCy ternary alloy layers”, Japanese J. Appl. Phys., 54, 04DH08 (2015).

[6] C. A. Stephenson, W. A. O'Brien, M. W. Penninger, W. F. Schneider, M. Gillett-Kunnath, J. Zajicek, K. M. Yu, R. Kudrawiec, R. A. Stillwell, M. A. Wistey, "Band structure of germanium carbides for direct bandgap silicon photonics", J. Appl. Phys., 120, 053102 (2016).