Ductile/brittle study of space craft materials by ab-initio electronic structure calculation.

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Abstract

In order to improve the ductility of high temperature structural materials namely cubic Rh_3B (where B= Ti, V) L_{12} intermetallic compounds, elastic properties of these compounds are computed for both pure and doped materials using the using Full Potential-Linearized Augmented Plane wave (FP-LAPW) method. Ternary addition is done with Vanadium, Hafnium and Aluminium. These materials are used in the design of gas turbine engine blades, solar probe space craft, etc.,. The elastic properties of cubic Rh_3Ti_x (V ,Hf,Al)$_{1-x}$ are computed for x=0, .125,.875,1 and are presented in the table

Covalent and brittle nature of the compounds could be decided based on (i) (C_{12}-C_{44}) values, G/B and √ values. i.e. when (C_{12}-C_{44}) is negative, G/B is >0.57 and when√ is < 0.26, the material is found to be brittle, otherwise it is ductile. Based on charge density plot also one can study the covalent nature of the given material. Based on Cauchy pressure values, it is inferred that pure Rh_3Ti is ductile and pure Rh_3V is brittle; for 12.5% titanium doped-Rh_3V, brittleness increases and for 12.5% vanadium doped-Rh_3Ti, the ductility decreases. In 12.5% Hafnium doped Rh3Ti, the ductility is better than that with vanadium. Further, instead oh Hafnium, if Rh3Ti is doped with 12.5% of Aluminium, it turns into brittle.It is proposed to extend the above study of electronic structure calculations by doping with other second, third and fourth group materials and it is under execution.

Parameters	**Rh_3V**	**$Rh_3V_{87.5}Ti_{12.5}$**	**Rh_3Ti**	**$Rh_3Ti_{87.5}V_{12.5}$**	**$Rh_3Ti_{87.5}Hf_{12.5}$**	**$Rh_3Ti_{87.5}Al_{12.5}$**
Lattice Constant (a.u.)	a_{exp}.=7.174 a_{cal}. =7.179	a_{opt}. = 14.378	a_{exp}.= 7.225 a_{cal}. = 7.269	a_{opt}. = 14.515	a_{opt}. = 14.586	a_{opt}. = 14.531
C_{11}	493.378	490.766	315.319	376.948	336.171	369.156
C_{12}	150.551	143.940	197.927	170.354	182.226	167.234
C_{44}	268.226	291.005	165.163	150.127	159.753	175.905
(C_{12}-C_{44})	-117.675	-147.065	32.764	20.227	22.473	-8.670
Bulk Modulus (B) GPa	264.827 at -0.046GPa	259.548 at 0.013GPa	237.058 at 0.067GPa	239.219 at -0.040GPa	233.5 at -0.046GPa	234. 542 at -0.047GPa
Shear Modulus (G) GPa	224.149	236.441	109.146	129.238	119.171	140.780
G/B	0.846	0.911	0.460	0.540	0.510	0.600
Poisson's Ratio	0.170	0.122	0.300	0.235	0.282	0.250