

Supplemental Material

A First-Principles Study on Mechanical and Thermodynamic Properties of $(\text{Nb}_{1-x}\text{Ti}_x)\text{C}$ Complex

Carbides Based on Virtual Crystal Approximation

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Table I lattice constants (a), elastic constants(C_{ij}), bulk modulus (B), shear modulus(G), Young's modulus (E) and Hardness of $(\text{Nb}_{1-x}\text{Ti}_x)\text{C}$ complex carbides

	a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)	Hardness (GPa)
NbC	4.517	629.2	126.6	161.5	294.1	192.9	474.9	22.04
		620 ¹	200 ¹	150 ¹	296 ²	200 ³	494 ³	18~24 ⁴
$(\text{Nb}_{0.75}\text{Ti}_{0.25})\text{C}$	4.511 ^v 4.491 ^c	608.8 ^v	125.8 ^v	173.6 ^v	286.8 ^v	198.2 ^v	483.3 ^v	22.85 ^v
		593.5 ^c	125.5 ^c	165.4 ^c	281.5 ^c	190.1 ^c	465.6 ^c	
$(\text{Nb}_{0.5}\text{Ti}_{0.5})\text{C}$	4.495 ^v 4.465 ^c	569.0 ^v	126.7 ^v	185.5 ^v	274.1 ^v	199.0 ^v	480.8 ^v	22.98 ^v
		551.0 ^c	123.1 ^c	174.0 ^c	265.7 ^c	189.0 ^c	458.4 ^c	
$(\text{Nb}_{0.25}\text{Ti}_{0.75})\text{C}$	4.464 ^v 4.438 ^c	517.3 ^v	124.7 ^v	191.4 ^v	255.6 ^v	193.3 ^v	463.2 ^v	22.11 ^v
		504.3 ^c	119.5 ^c	176.2 ^c	247.8 ^c	182.5 ^c	439.6 ^c	
TiC	4.411	457.1	112.1	168.8	227.1	170.3	408.7	18.7
		500 ⁵	113 ⁵	175 ⁵	240 ²	187 ³	454 ³	18~23 ⁴

Note: the superscript (v) denotes the data are calculated with virtual crystal approximation, (c) denotes the data are calculated based on cubic cell, the superscript number, from (1) to(5), denote the data are cited from ref.(1) to(5), respectively

Table II the ideal tensile strength (ITS), σ_{max} , the ideal shear strength(ISS), τ_{max} , the tensile strain energy density (W_{tensile}), the shear strain energy density (W_{shear}), the reciprocal of brittleness (β^{-1}) and the fracture toughness (K_{IC}) of $(\text{Nb}_{1-x}\text{Ti}_x)\text{C}$ complex carbides

	σ_{max} (GPa)	τ_{max} (GPa)	W_{tensile} (GPa)	W_{shear} (GPa)	β^{-1}	K_{IC} (MPa·m ^{1/2})
NbC	72.4	28.4	19.5	4.8	4.073	4.981
						2.0~3.0 ⁶
						3.0~4.0 ⁴
$(\text{Nb}_{0.75}\text{Ti}_{0.25})\text{C}$	79.1	29.0	21.4	4.9	4.336	5.275
$(\text{Nb}_{0.5}\text{Ti}_{0.5})\text{C}$	83.4	28.6	22.5	4.9	4.605	5.473
$(\text{Nb}_{0.25}\text{Ti}_{0.75})\text{C}$	84.8	27.5	22.8	4.6	4.925	5.587
TiC	83.3	25.6	21.6	4.1	5.229	5.366
						2.0~4.0 ⁷
						3.5~4.3 ⁴

Note: the superscript number (4) , (6) and (7) denote the data are cited from ref.(4) ,(6) and (7), respectively

Reference

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