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Ab initio study of metal carbide hydrides in 2.25Cr1Mo0.25V steel

Min He,[a] Chidozie Onwudinanti,[b] Yaoting Zheng,[c] Xiaomei Wu,[a] Zaoxiao Zhang*[a] and Shuxia Tao*[d]

[a] *State Key Laboratory of Multiphase Flow in Power Engineering, School of Chemical Engineering and Technology, Xi'an Jiaotong University, No.28, Xianning West Road, Xi'an, Shaanxi, 710049, P.R. China. E-mail: zhangzx@xjtu.edu.cn*

[b] *Center for Computational Energy Research, DIFFER - Dutch Institute for Fundamental Energy Research De Zaale 20, 5612AJ Eindhoven, The Netherlands.*

[c] *School of science, Xi'an University of Architecture and Technology, No.13, Yanta Road, Xi'an Shaanxi, 710055, P.R. China.*

[d] *Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands. E-mail: s.x.tao@tue.nl*

Table S 1 Basic calculation parameters and per atom energy of metal-carbon systems.

	Space group	Lattice parameters [Å]	E_{cut} [eV]	K-mesh	E_M [eV]	ΔE_f [eV]
C(diamond)	Fd3m	2.53×2.53×2.53	500	8×8×8	-9.09	
C(graphite)	$P6_3/mmc$	2.47×2.47×7.91	500	8×8×2	-9.22	
Cr	Im3m	2.85×2.85×2.85	500	8×8×8	-9.51	
Mo	Im3m	3.16×3.16×3.16	400	10×10×10	-10.92	
V	Im3m	3.00×3.00×3.00	500	10×10×10	-8.96	
$Cr_{23}C_6$	$Fm\bar{3}m$	10.54×10.54×10.54	700	2×2×2		-0.09
Cr_7C_3	Pnma	4.50×6.88×12.09	700	5×3×2		-0.16
Cr_7C_3	$P6_3mc$	13.87×13.87×4.49	700	2×2×10		-0.12
CrC	$Fm\bar{3}m$	4.06×4.06×4.06	450	8×8×8		0.17
Mo_2C	Pbcn	4.74×6.06×5.22	800	12×12×12		-0.15
MoC	$P\bar{6}m2$	2.92×2.92×2.82	800	9×9×9		-0.13
MoC	$Fm\bar{3}m$	4.37×4.37×4.37	500	8×8×8		0.16
V_2C	$P6_3/mmc$	2.89×2.89×4.53	450	10×10×5		-0.46
V_2C	Pbcn	4.55×5.73×5.04	450	8×8×8		-0.48
V_3C_2	$R\bar{3}m$	2.92×2.92×27.80	450	8×8×1		-0.41
V_4C_3	$Fm\bar{3}m$	4.12×4.12×4.12	500	8×8×8		-0.34
V_6C_5	$P3_112$	5.10×5.10×14.36	500	10×10×2		-0.55
V_8C_7	$P4_132$	8.34×8.34×8.34	500	6×6×6		-0.53
VC	$Fm\bar{3}m$	4.16×4.16×4.16	500	8×8×8		-0.41

Table S 2 The formation enthalpies and hydrogen formation enthalpies of metal carbides in the original, compressed and tense lattices.

Stress	$\triangle E_f$ [eV]			$\triangle E_H$ [eV]		
	Cr_7C_3	Mo_2C	V_6C_5	$(Cr_7C_3)_4H$	$(Mo_2C)_{16}$ H	$(V_6C_5)_3H$
Origin	-0.163	-0.150	-0.548	0.496	0.146	-0.131
Compressed	0.161	0.160	-0.350	1.314	0.602	-0.041
Tense	0.061	0.060	-0.412	-0.091	-0.131	-0.081

Above we report the results of calculations to study the effect of strain on metal carbide hydrogen absorption, in Table S2. The original structure is the relaxed lattice structure, the compressed structure has a lattice constant 95% of the original, and the tensile structure is extended to 105%. It can be observed that the strain raises the formation enthalpy for the carbides; both compression and tension change the formation enthalpy of Cr_7C_3 and Mo_2C from negative to positive, while that of V_6C_5 remains negative, albeit higher.

The hydride formation enthalpies of all three metal carbides increase in the compressed state, with V_6C_5 hydride maintaining a (slightly) negative formation energy. Cr_7C_3 and Mo_2C hydride formation energies decrease to negative values in tense state. Notably the case for V_6C_5 is the opposite, although the formation energy remains negative despite its rise. The conclusion is that compressive strain will decrease both the stability and the hydrogen absorption ability of the metal carbides, while tensile strain

will decrease the stability of metal carbides, but increase hydrogen absorption ability of the metal carbides in the alloy, with the exception of vanadium carbide.