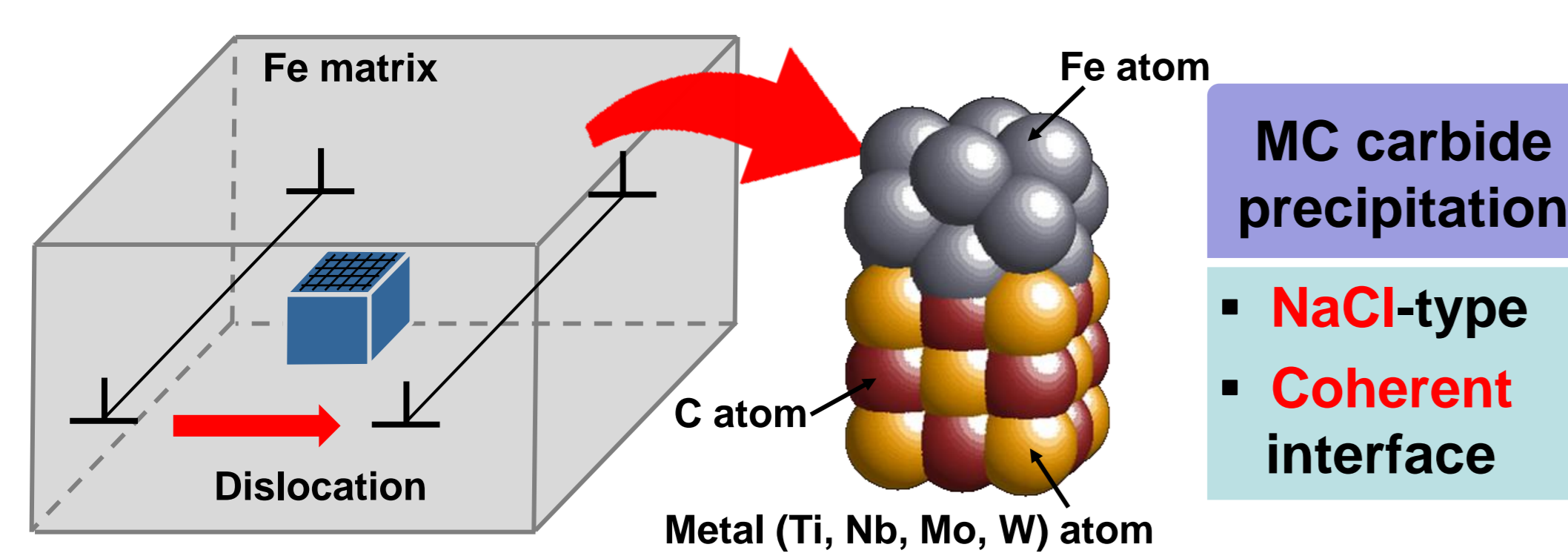


Introduction

NaCl-type MC carbides are one of the most important precipitates for strengthening steels. To obtain desired materials properties, it is necessary to understand the precipitation behavior of carbides and the interaction between precipitates and various defects such as dislocations or grain boundaries. As a means to enable an atomic-level investigation on the behavior of MC carbides, in the present study, the second nearest-neighbor modified embedded-atom method (2NN MEAM) interatomic potential for Fe-Metal-C (Metal: Ti, Nb, Mo, W) ternary systems and constituent binary Fe-Metal and Metal-C systems are developed. It is shown that the potentials reproduce various fundamental physical properties of relevant systems reasonably well.

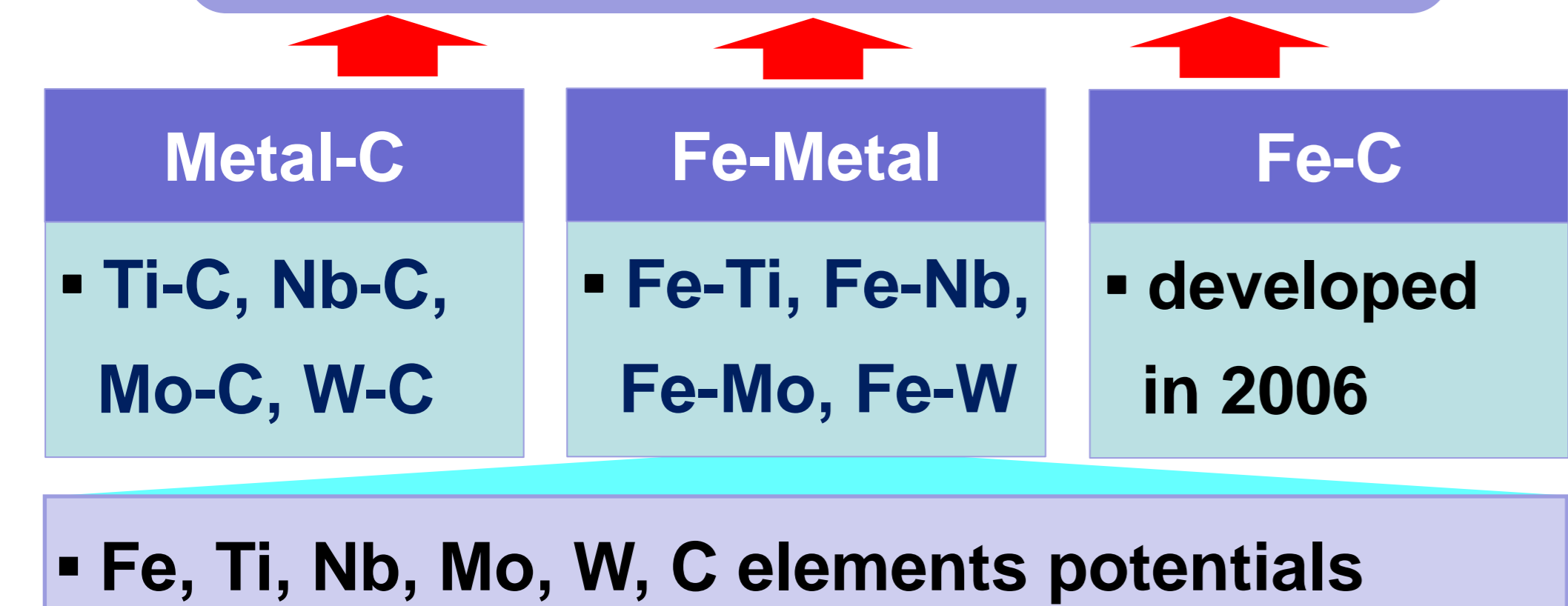
Development of (2NN MEAM) interatomic potentials

1 Background and Object

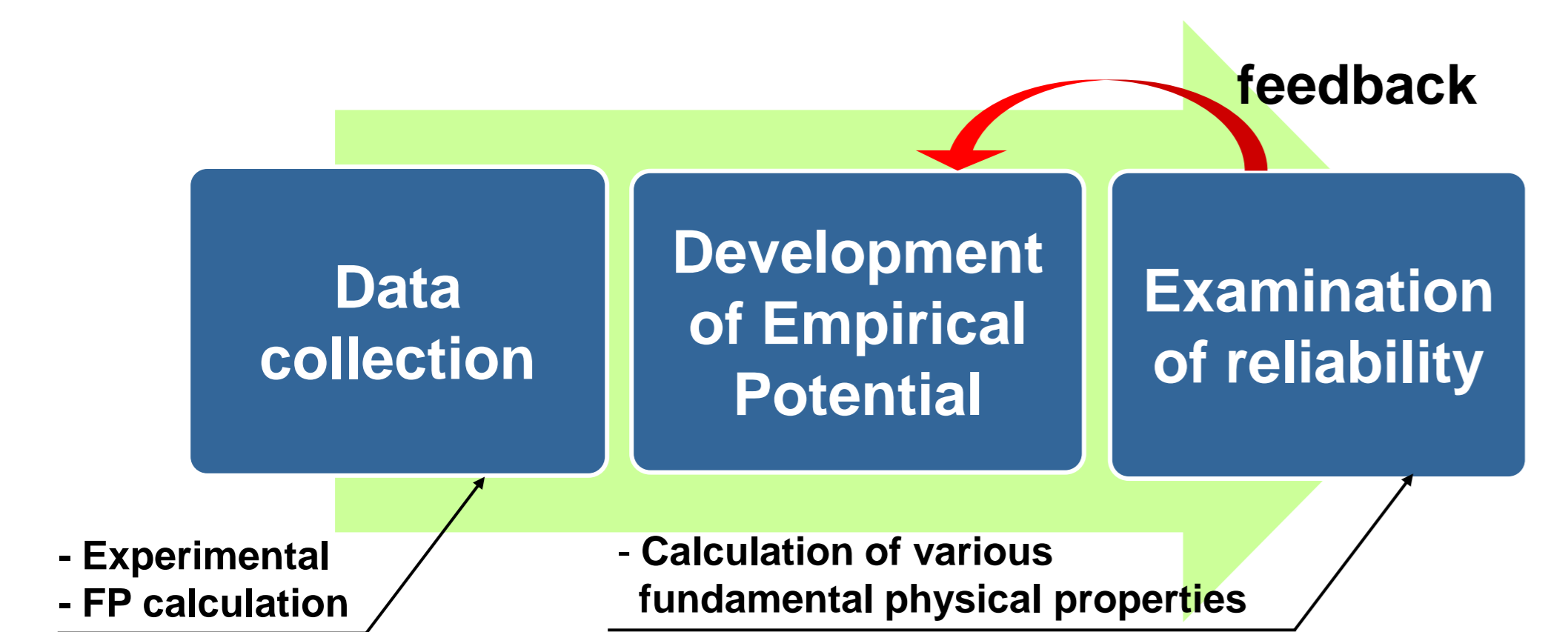


1. Interfacial properties between Fe matrix and NaCl-type carbides
2. Dislocation-precipitation interaction

Fe-Metal-C (Metal=Ti, Nb, Mo, W)
2NN MEAM interatomic potentials



2 Method of development of potentials



3 Metal-C (Ti, Nb, Mo, W) binary systems

Lattice parameter & Enthalpy of formation

Type	Properties	MEAM	Exp.	FP Calculations
Ti-C (NaCl-type)	Lattice constant, a	4.420	4.330, 4.329, 4.326, 4.317	4.38, 4.348, 4.341, 4.316, 4.345, 4.343, 4.315, 4.33
	Enthalpy of formation	-0.78	-0.78	-
Nb-C (NaCl-type)	Lattice constant, a	4.560	4.430, 4.469, 4.470, 4.4707, 4.471	4.43, 4.45, 4.476, 4.489, 4.49
	Enthalpy of formation	-0.730	-0.729±0.013, -0.731, -0.729, -0.701, -0.721	-0.585
	Nb ₂ C (hex)	Lattice constant, a, c	3.218, 5.104	3.119, 3.122, 4.959, 4.964
Mo-C (NaCl-type)	Lattice constant, a	4.44	4.278	4.366, 4.278, 4.42, 4.33, 4.316
	Enthalpy of formation	0.183	0.0056	0.082, 0.136
	MoC (hex)	Lattice constant, a, c	2.979, 2.999	-
W-C (NaCl-type)	Lattice constant, a	4.48	4.192, 4.221, 4.266	4.482, 4.29, 4.32
	Enthalpy of formation	-0.02	-0.02	-
	WC (hex)	Lattice constant, a, c	3.018, 2.920	2.837, 2.84
Enthalpy of formation	-0.16	-0.21	-	-

※ The units of the lattice parameter and enthalpy of formation are Å and eV atom⁻¹.

Elastic constant

Properties	TiC (NaCl-type)			NbC (NaCl-type)		
	MEAM	Exp.	FP Calculations	MEAM	Exp.	FP Calculations
Bulk modulus B	2.42	2.41, 2.42	2.67, 2.47, 2.75, 2.44, 2.2, 2.52, 2.14	3.40	2.96, 3.02, 3.40	2.93, 2.99, 3.01, 3.06
Elastic constant C ₁₁	5.22	5.00, 5.13	4.91, 6.10, 6.06, 4.7	5.49	6.20	5.46, 6.27, 6.4, 6.67
C ₁₂	1.02	1.13, 1.06	1.20, 1.24, 1.06, 0.97	2.35	2.00	1.67, 1.79, 1.8, 1.63
C ₄₄	1.29	1.75, 1.78	1.89, 1.73, 2.3, 1.67	1.73	1.50	2.24, 2.20, 1.4, 1.61

※ The units of elastic constants B, C₁₁, C₁₂, C₄₄ are 10¹²dyne/cm².

Surface energy

Surface	MEAM		FP Calculation	
	MEAM	FP Calculation	MEAM	FP Calculation
TiC (100) (NaCl-type)	2.91	1.665, 2.254, 1.73, 1.71	3.40	2.96, 3.02, 3.40
(110)	3.76	3.631, 3.78	3.40	2.96, 3.02, 3.40
(111)	4.05	3.122, 5.63	3.40	2.96, 3.02, 3.40
NbC (100) (NaCl-type)	2.46	2.81	3.40	2.96, 3.02, 3.40
(110)	2.65	-	3.40	2.96, 3.02, 3.40
(111)	2.47	-	3.40	2.96, 3.02, 3.40

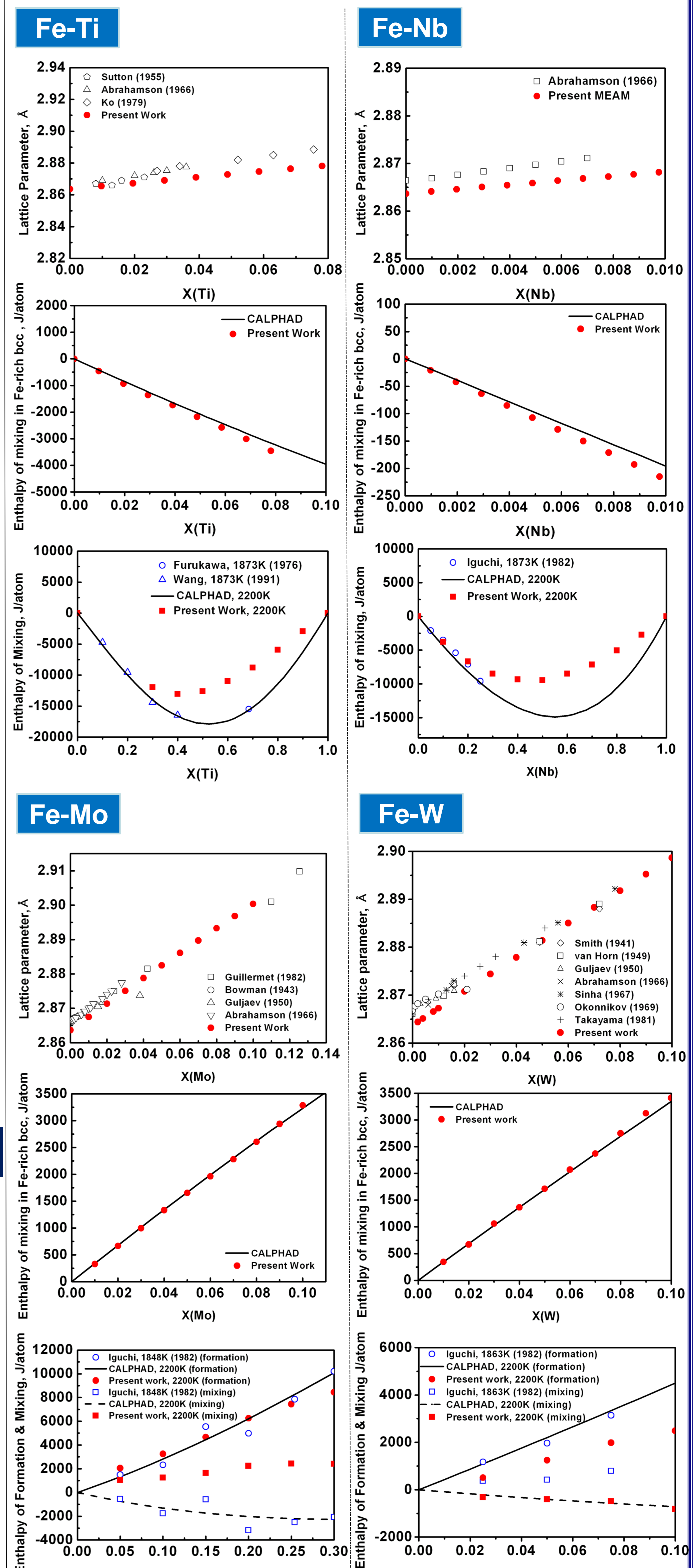
※ The unit of surface energy is J/m².

Dilute heat of solution

Surface	MEAM	Exp.*
In hcp Ti	-1.05	-1.4
In bcc Nb	0.44	-0.22
In bcc Mo	1.77	0.97
In bcc W	1.82	1.30

※ The unit of dilute heat of solution is eV. * Thermodynamic assessment

4 Fe-Metal (Ti, Nb, Mo, W) binary systems

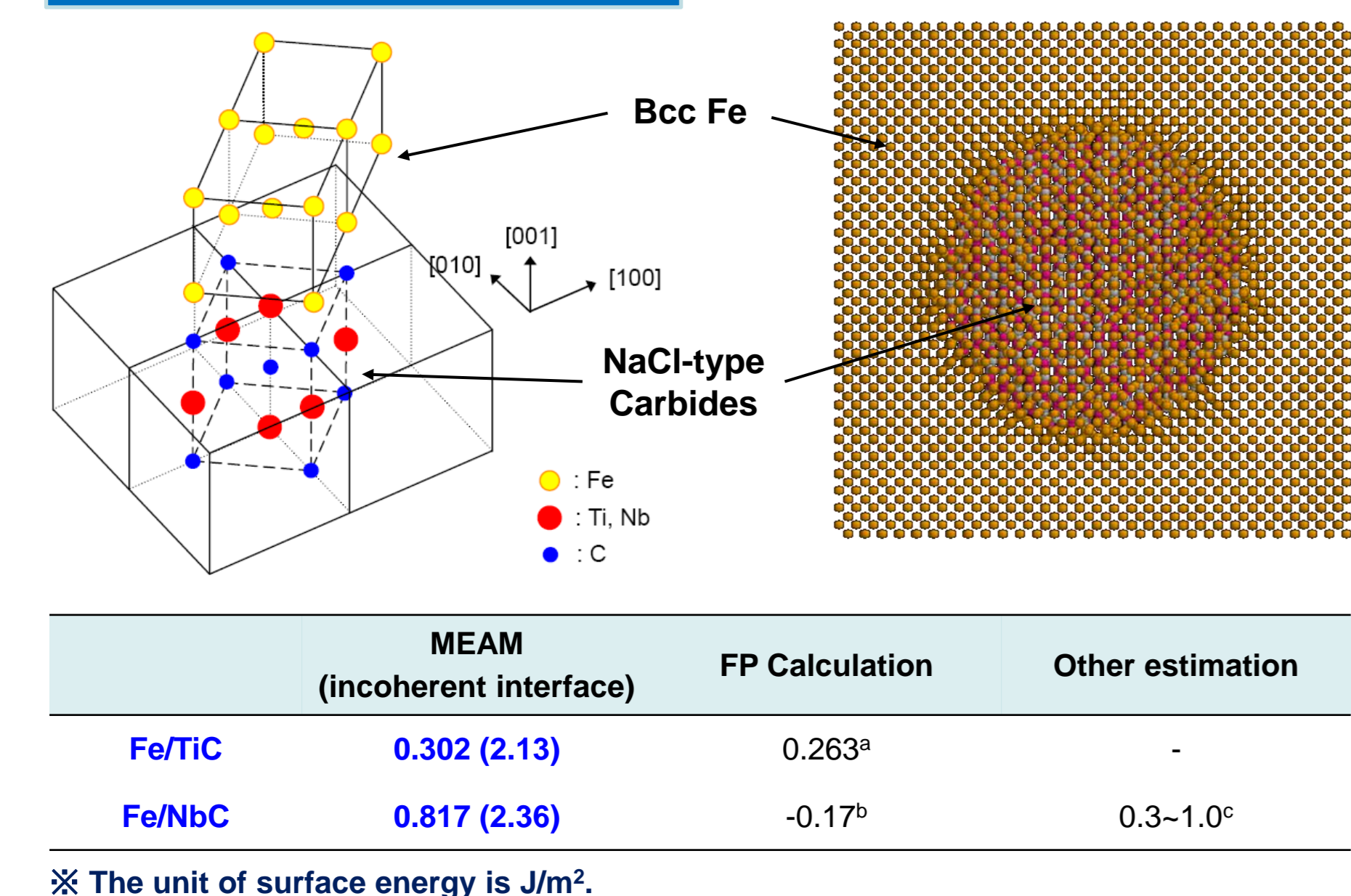


The reasonable agreement between the present calculation and literature information on the relevant binary systems

5 Fe-Metal-C (Ti, Nb, Mo, W) ternary systems

- The ternary parameters could be automatically determined from potential parameters for constituent binary systems.

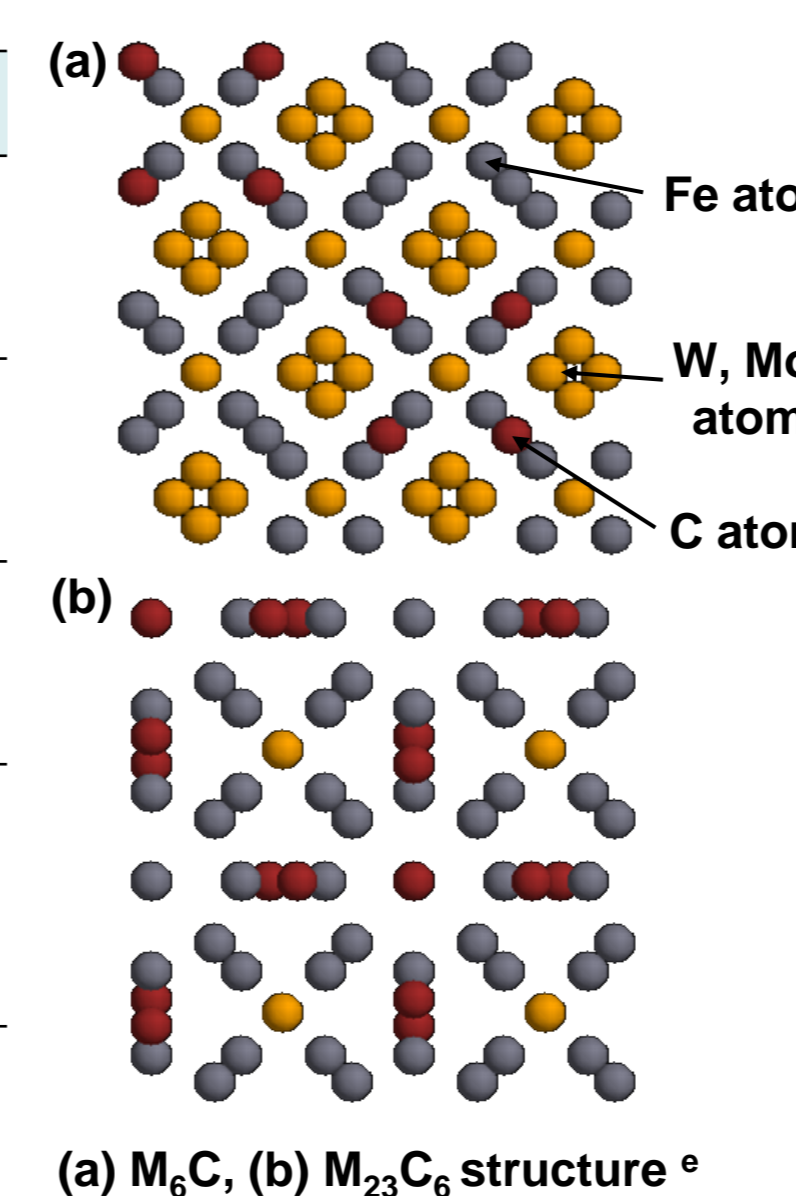
Fe-Ti-C & Fe-Nb-C



Fe-Mo-C & Fe-W-C

Type	Properties	MEAM	Exp. ^d
M ₃ C (Fe ₃ W ₃ C)	Lattice constant, a	unstable	11.087
	Enthalpy of formation	-	-0.072
Fe-W-C (M ₂₃ C ₆ (Fe ₂₁ W ₂ C ₆))	Lattice constant, a	10.518	10.52
	Enthalpy of formation	-0.061	0.077
M ₃ C (Fe ₃ Mo ₃ C)	Lattice constant, a	unstable	11.08
	Enthalpy of formation	-	-0.154
Fe-Mo-C (M ₂₃ C ₆ (Fe ₂₁ Mo ₂ C ₆))	Lattice constant, a	10.529	10.54, 10.53, 10.52
	Enthalpy of formation	-0.057	0.038

※ The units of the lattice parameter and enthalpy of formation are Å and eV atom⁻¹.



Conclusions

It has been shown that the present 2NN MEAM potentials for the relevant systems can reproduce various fundamental physical properties - structural properties (enthalpy of formation, lattice parameter and dilute heat of solution), elastic properties (bulk modulus, elastic constants) and surface energy. The present potentials can be applied to atomic-level investigations of the precipitation behavior of Metal-C (Metal:Ti, Nb, Mo, W) carbides and their effects on the deformation and mechanical properties of steels.

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