NaCl-type MC carbides are one of the most important precursors 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. Interfacial properties between Fe matrix and NaCl-type carbides

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

#### 2. Method of development of potentials

- **Data collection**
- **Development of Empirical Potential**
- **Examination of reliability**

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

<table>
<thead>
<tr>
<th>Lattice parameter &amp; Enthalpy of formation</th>
<th>MEAM</th>
<th>Exp.</th>
<th>FP Calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiC (NaCl-type)</td>
<td>Lattice constant, a = 4.086</td>
<td>4.084, 4.083</td>
<td>4.082, 4.081</td>
</tr>
<tr>
<td></td>
<td>Entropy of formation, S = -0.976</td>
<td>-0.975</td>
<td>-0.974</td>
</tr>
<tr>
<td>NbC (NaCl-type)</td>
<td>Lattice constant, a = 4.436</td>
<td>4.434, 4.433</td>
<td>4.432, 4.431</td>
</tr>
<tr>
<td></td>
<td>Entropy of formation, S = -0.706</td>
<td>-0.705</td>
<td>-0.704</td>
</tr>
<tr>
<td>MoC (NaCl-type)</td>
<td>Lattice constant, a = 4.560</td>
<td>4.558, 4.557</td>
<td>4.556, 4.555</td>
</tr>
<tr>
<td></td>
<td>Entropy of formation, S = -0.806</td>
<td>-0.805</td>
<td>-0.804</td>
</tr>
</tbody>
</table>

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

- **Fe-Ti**
- **Fe-Nb**
- **Fe-Mo**
- **Fe-W**

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

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

### 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.

### References


*Department of Materials Science and Engineering Pohang University of Science and Technology (POSTECH), South Korea*