**Development of Embedded-Atom Method (EAM) Potential for Palladium-Barium Alloy**

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**Codes for using the EAM potential in LAMMPS:**

In the interatomic potential section of the LAMMPS code, the below two lines must be given -

>>pair\_style eam/alloy

>>pair\_coeff \* \* BaPd\_SPSM.EAM Ba Pd

The name of the developed EAM potential file is ‘BaPd\_SPSM\_EAM.txt’. The file extension should be ‘.EAM’ while using this in the LAMMPS code. The elements are Barium (Ba) and Palladium (Pd).

**Diffusion coefficients at low temperatures:**

Diffusion coefficients for Ba, Pd, and BaPd2 at 77K, and 87Kare listed in TABLE VI.

|  |  |  |  |
| --- | --- | --- | --- |
| T (K) | D\_Ba ( m2/s ) | D\_Pd ( m2/s ) | D\_BaPd2 ( m2/s ) |
| 77 | 3.664×10-12 | 2.946×10-12 | 2.637×10-12 |
| 87 | 3.810×10-12 | 4.207×10-12 | 3.864×10-12 |

**TABLE VI –** Data of diffusion coefficient (D) for 77K, and 87K.