References for Potential and Functional Models

Pair Potentials:

GENERAL (but old)

1) "Interatomic Potentials" by Ian Torrens, Academic Press (1972) *This is a good book but old. The specific information on energy models is not up to data, but it may be used as a general introduction*

OXIDES:

2) G.V. Lewis and C R A Catlow, J. Phys. C: Solid State Phys, **18** (1985), 1149

3) T. S. Bush, J. D. Gale, R. A. Catlow, P. D. Battle, *Journal of Materials Chemistry* **4**, (1994) 831-837

ORGANIC MATERIALS:

4) "Introduction to Computational Chemistry", Frank Jensen, Wiley. This is a very good book. The Second chapter deals in detail with the potential forms used in organic chemistry. The remaining chapters deal with ab initio and semi-empirical methods. **Highly Recommended**

5) reading about the Cauchy relation (C12=C44) for pair potentials: "Dynamical Theory of Crystal Lattices", M Born and K, Huang, Oxford Classic Texts, p139.

Stillinger-Weber

6) F.H. Stillinger and T.A. Weber, Phys. Rev. B, **31**, 5262 (1985).

Multi-body Interactions

7) A good book to read is: "Many-Atom Interactions in Solids" ed. R.M. Nieminen, M.J. Puska and M.J. Manninen, Springer-Verlag, Proceedings in Physics Vol 48 (1990).

8) An excellent review paper on the need to go beyond pair potentials is: A.E. Carlsson, "Beyond Pair Potentials in Elemental Transition Metals and Semiconductors", Solid State Physics, ed Ehrenreich and Turnbull, **43**, 1-91 (1990).

EAM Papers

9) M.S.Daw, S.M. Foiles and M.I. Baskes, "The embedded-atom method: a review of theory and applications", Materials Science Reports, **9**, 251-310 (1993). **Highly Recommended.**

10) M.S. Daw, Phys. Rev. B, **39**, 7441 (1989).

These papers contain references to many of the other EAM papers

11) A more general description of the Effective Medium Theory can be found in: K.W. Jacobsen, "Bonding in Metallic Systems: An Effective Medium Approach", Comments in Con. Mat. Phys., **14**, 129-161 (1988).

12) FINNIS-SINCLAIR: M.W. Finnis and J.E. Sinclair, "A simple empirical N-body potential for transition metals", Phil. Mag A, **50**, 45-55 (1984).

13) For a comparison between the different various of **effective medium potentials**: T.J. Raeker and A.E. DePristo, "Intern. Rev. Phys. Chem. **93**, 1 (1991).

14) A series of overview articles on empirical energy methods can be found in the February 1996 issue of the **MRS Bulletin**.

Some of the potentials used for Si in the literature:

1) Keating:
P.N.Keating,Phys.Rev. 145,637(1966)
Valid only for small deviations from the ideal diamond lattice sites. Used for elastic constants and phonon properties.

2) Stillinger-Weber:
F.H.Stillinger and T.A. Weber, Phys. Rev. B 31, 5262 (1985) 2 and 3 body terms. Fitted to stable crystal structure, reasonable melting temperature and g(r) in the liquid.

3) Tersoff:
J. Tersoff, Physical Review B, vol.38, (no.14):9902-5 (1988) pair functional. gets good elastic properties, stable crystal structures, liquid properties.

4) Biswas-Hamann
R. Biswas and D.R. Hamann, Phys.Rev.Lett. 55,2001(1985)
R. Biswas and D.R. Hamann, Phys.Rev.B 36, 6434 (1987)
Rather complicated to evaluate. Two versions. The first is longer ranged than the second. The old one is better at bulk metallic Si phases and high pressure transitions of Si. The new one does better for layered and interstitial structures.

5) Embedded Atom
M.I.Baskes, Phys.Rev.Lett. 59,2666(1987)
Modification of the EAM of metals to deal with covalent bonding, including
and angle-dependent electron density to model the effects of bond bending.
Fitted to Si lattice constant, sublimation energy and elastic constants.
Reproduces well the LDA structural geometries and energies.

6) Kaxiras-Pandey Kaxiras, E.; Pandey, K.C., Physical Review B vol.38, 12736 (1988)
2 and 3 body fitted to self diffusion paths in pure silicon. Suited
for molecular dynamics simulations of atomic processes in Si.

Others:
- Pearson, Takai, Halicioglu and Tiller, J.Cryst.Growth 70,33(1984)
- Dodson, Phys.Rev.B 35,2795(1987)
- Khor and Das Sarma, Several articles in PRB 1988-89.
- Chelikowsky, J.R.; Phillips, J.C.; Kamal, M.; Stauss, M.,
  Phys Rev Lett 62, 292(1989)

A comparison between 6 of these potentials can be found in Balamane, H.; Halicioglu, T.; Tiller, W.A. Comparative study of silicon empirical interatomic potentials. Physical Review B 46,2250 (1992)

For a review and comparison of valence force field potentials (i.e., potentials that only describe small displacements from the ideal sites, like the Keating potential), see Stoneham, A.M.; Torres, V.T.B.; Masri, P.M.; Schober, H.R.
Philosophical Magazine A 58,93 (1988)
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