Supporting Information

Mechanism of Hydrogen-accelerated Melting of Polycrystalline Copper

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TABLE S1: Lattice constants a, c (in unit of Å), bulk moduli B (in unit of GPa), cohesive energies E_c (in unit of kcal mol^{-1}) and relative energy ΔE (in unit of kcal mol^{-1}) for different phases of Cu.

		ReaxFF	DFT	Expt.
fcc	a	3.61	3.63	3.61[a]
	B	122.43	131.28	137.8[b]
	E_c	80.39	80.31	81.2[c]
	ΔE	0.00	0.00	–
bcc	a	2.88	2.89	–
	B	109.43	129.48	–
	E_c	79.54	79.45	–
	ΔE	0.86	0.86	–
a15	a	4.59	4.62	–
	B	112.15	123.36	–
	E_c	77.75	78.07	–
	ΔE	2.64	2.24	–
ac	a	2.38	2.41	–
	B	119.64	95.75	–
	E_c	69.02	69.68	–
	ΔE	11.38	10.63	–
dia	a	5.32	5.36	–
	B	47.32	50.42	–
	E_c	40.71	56.67	–
	ΔE	39.68	23.64	–
hcp	a	2.55	2.57	–
	c	4.16	4.20	–
	B	120.16	129.78	–
	E_c	80.28	80.13	–
	ΔE	0.12	0.18	–

[a] Reference 1.

[b] Reference 2.

[c] Reference 3.

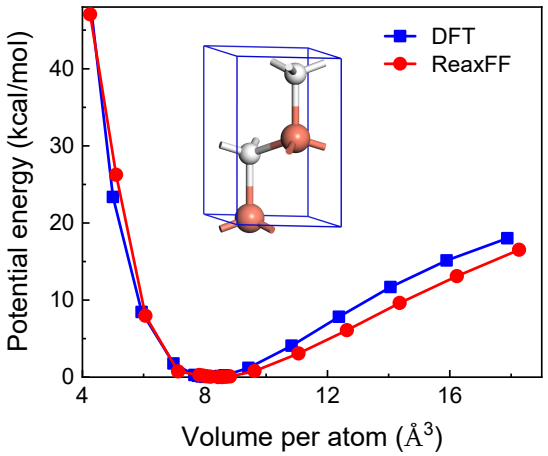

Figure S1. Equations of states calculated by ReaxFF and DFT for the hexagonal wurtzite type structure of CuH belonging to the space group $P6_3mc$.

TABLE S2: Lattice constants a, c (in unit of Å), formation enthalpy E_f (in unit of kcal mol^{-1}) for different phases of copper hydride crystals.

Composition	Space group		ReaxFF	DFT	Other DFT	Expt.
HCu	$Fm\bar{3}m$	a	3.87	3.89	3.90[a]	3.7[b]
		E_f	1.35	5.76	–	–
HCu	$Pm\bar{3}m$	a	2.64	2.50	–	–
		E_f	16.93	13.29	–	–
HCu	$F\bar{4}3m$	a	4.03	4.02	4.02[a]	–
		E_f	2.92	3.11	–	–
HCu	$P6_3mc$	a	2.89	2.87	2.89[a]	2.90[c]
		c	4.60	4.57	4.57[a]	4.60[c]
		E_f	2.96	2.99	–	–
H_2Cu	$Fm\bar{3}m$	a	2.90	3.04	–	–
		E_f	10.96	9.66	–	–
H_2Cu	$Pa\bar{3}$	a	4.10	4.29	–	–
		E_f	10.97	9.66	–	–
H_2Cu	$Pn\bar{3}m$	a	3.65	3.72	–	–
		E_f	7.08	13.07	–	–
H_2Cu	$P4_2/mnm$	a	4.78	4.78	–	–
		c	2.40	2.40	–	–
		E_f	11.94	6.39	–	–

[a] Reference 4.

[b] Reference 5.

[c] Reference 6.

Force Field developed in this study

Cu/H ReaxFF reactive force field H. S. Huang et al.

39 ! Number of general parameters

50.0000 ! Overcoordination parameter

9.5469 ! Overcoordination parameter

1.6725 ! Valency angle conjugation parameter

1.7224 ! Triple bond stabilisation parameter

6.8702 ! Triple bond stabilisation parameter

60.4850 ! C2-correction

1.0588 ! Undercoordination parameter

4.6000 ! Triple bond stabilisation parameter

12.1176 ! Undercoordination parameter

13.3056 ! Undercoordination parameter

-40.0000 ! Triple bond stabilization energy

0.0000 ! Lower Taper-radius

10.0000 ! Upper Taper-radius

2.8793 ! Not used

33.8667 ! Valency undercoordination

6.0891 ! Valency angle/lone pair parameter

1.0563 ! Valency angle

2.0384 ! Valency angle parameter

6.1431 ! Not used

6.9290 ! Double bond/angle parameter

0.3989 ! Double bond/angle parameter: overcoord

3.9954 ! Double bond/angle parameter: overcoord

-2.4837 ! Not used

5.7796 ! Torsion/BO parameter

10.0000 ! Torsion overcoordination

1.9487 ! Torsion overcoordination

-1.2327 ! Conjugation 0 (not used)

2.1645 ! Conjugation

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   1.5591 ! vdWaals shielding
   0.1000 ! Cutoff for bond order (*100)
   1.7602 ! Valency angle conjugation parameter
   0.6991 ! Overcoordination parameter
  50.0000 ! Overcoordination parameter
   1.8512 ! Valency/lone pair parameter
   0.5000 ! Not used
  20.0000 ! Not used
   5.0000 ! Molecular energy (not used)
   0.0000 ! Molecular energy (not used)
 0.7903 ! Valency angle conjugation parameter
  2    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;
         alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
         cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
         ov/un;val1;n.u.;val3,vval4
 H    0.9479   1.0000   1.0080   1.1364   0.0232   0.9900  -0.1000   1.0000
      9.0643   4.7746   1.0000   0.0000 121.1250   4.7757   9.7732   1.0000
     -0.1000   0.0000  62.4879   2.5194   2.3785   0.2223   1.0698   0.0000
    -15.7683   2.1488   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 Cu   1.9771   2.0000  63.5460   1.6202   0.2741   1.0000   0.1000   1.0000
     13.7875   4.7439   1.0000   0.0000   0.0000   2.9838   6.0000   0.0000
     -1.0000   0.0000  80.7000  34.9555   0.4988   0.0000   0.8563   0.0000
     -0.1243   3.1491   1.0000   4.0000   2.5791   0.0000   0.0000   0.0000
  3    ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                  pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
  1  1 113.9232   0.0000   0.0000  -0.5971   0.0000   1.0000   6.0000   0.9093
        1.7152   1.0000   0.0000   1.0000  -0.0450   6.0710   0.0000   0.0000
  2  2  26.4159   0.0000   0.0000   0.7357  -0.2000   0.0000  16.0000   0.3169
        0.2678  -0.2000  15.0000   1.0000  -0.1593   4.1024   0.0000   0.0000
  1  2  47.0693   0.0000   0.0000   0.9599   0.0000   1.0000   6.0000   0.3591
        0.0204   1.0000   0.0000   1.0000  -0.0710   7.9806   0.0000   0.0000
  1    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
```

1 2 0.9999 0.8942 14.9978 1.9994 -1.0000 -1.0000

5 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2

1 1 1 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400

1 2 1 89.0363 5.0589 4.8604 0.0000 0.8141 0.0000 1.4290

1 1 2 59.7817 20.1663 1.5872 0.0000 2.8343 0.0000 1.3764

2 1 2 4.9491 5.7486 7.2109 0.0000 0.3755 0.0000 1.5182

1 2 2 43.6373 1.2986 6.1920 0.0000 1.4977 0.0000 4.6641

0 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n

0 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1

References

1 N. Jakse and A. Pasturel, *Phys. Rev. Lett.*, 2003, **91**, 195501.

2 W. F. Gale and T. C. Totemeier, Smithells Metals Reference Book 8th Edn, (Butterworth-Heinemann, Oxford, 2004).

3 K. Kambe, *Phys. Rev.*, 1955, **99**, 419.

4 Y. G. Li and P. A. Korzhavyi, *Dalton. T.*, 2017, **46**, 529.

5 R. Burtovyy and M. Tkacz, *Solid. State. Commun.*, 2004, **131**, 169.

6 P. A. Korzhavyi, I. L. Soroka, E. I. Isaev, C. Lilja, and B. Johansson, *Proc. Natl. Acad. Sci.*, 2012, **109**, 686.