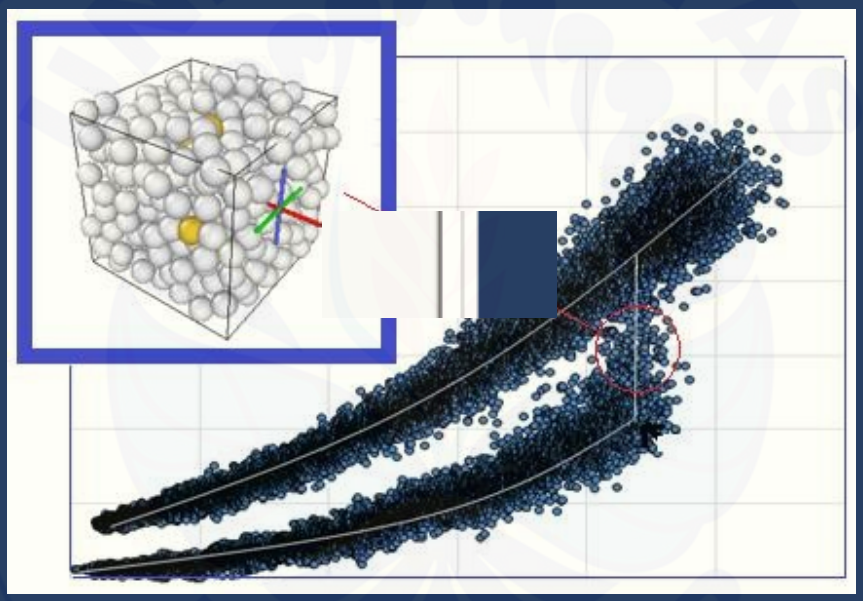
Artoto Arkundato
Moh. Hasan
Zaki Su'ud

Fisika Komputasi

Simulasi Dinamika Molekul dan Aplikasinya



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Fisika Komputasi

Simulasi Dinamika Molekul dan Aplikasinya

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Artoto Arkundato
Moh. Hasan
Zaki Su'ud

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PRAKATA

Alhamdulillah, buku teks hasil riset ini akhirnya berhasil kami susun setelah melalui proses pembuatan, editing dan perbaikan dan revisi dalam yang cukup lama. Buku ini diharapkan dapat memberikan bahan atau referensi tambahan untuk mendukung riset yang menggunakan Metode Dinamika Molekul. Buku ini juga diharapkan dapat memberi bekal bagi yang tertarik mempelajari metode dinamika molekul untuk pengembangan riset/penelitian baik bidang fisika, kimia, biologi dan matematika bahkan tidak menutup kemungkinan pada bidang farmasi dan ilmu bahan. Metode dinamika molekul sebagai salah satu metode komputasi yang handal, dewasa ini mempunyai tempat dan peran yang sangat penting bagi kemajuan ilmu dan penegmbangan teknologi. Banyak berbagai fenomena bidang sains yang dapat diprediksi gejala dan prosesnya melalui pendekatan metode dinamika molekul. Dengan makin meningkat pesatnya sumber daya komputasi seperti kecepatan processor komputer, kemampuan memori komputer, teknologi jaringan komputer, kapasitas dan kemampuan media penyimpan data maka penerapan metode dinamika molekul untuk menangani problem-problem kompleks bidang sains dan teknik menjadi semakin memungkinkan dan menjanjikan. Dengan memodelkan sistem material dan mensimulasikan fenomena yang terkait yang ingin diteliti maka pencapaian-pencapaian dan inovasi-inovasi bidang sains dapat dimaksimalkan dengan penggunaan sumber dana yang efisien.

Buku Teks ini telah mengalami revisi dari edisi pertama (tahun 2016) dengan memasukkan hasil-hasil Riset Hibah Terapan DRPM 2021, khususnya pada modul 1, 2, 4 dan 5 serta Lampiran, dimana berbagai aspek dan data penting telah ditambahkan menyesuaikan dengan kebutuhan simulasi. Buku ini secara umum dapat juga digunakan sebagai bahan rujukan oleh mahasiswa yang melakukan penelitian tugas akhir/thesis/disertasi bidang komputasi material. Namun demikian buku ini juga ada manfaatnya jika digunakan untuk bahan rujukan perkuliahan fisika komputasi. Apa yang menjadi kekhasan dari buku ini adalah pembaca akan dibawa mendalami mulai dari tingkatan dasar, diberikan pendangan yang cukup mengenai urgensi dari metode komputasi, diberikan cara bagaimana bagi pemula untuk memasuki metode komputasi ini baik berkenaan dengan sistem operasi, instalasi, software-software yang diperlukan, sampai bagaimana menjalankan program simulasi yang mana lebih ditekankan pada persiapan melakukan riset di bidang komputasi material. Software-software yang digunakan juga software-software yang popular digunakan dalam riset komputasi material yang hasil-hasilnya banyak dipublikasikan dalam jurnal dan prosidings internasional.

Akhirnya tentu saja tidak ada yang sempurna kecuali Gusti Allah azza wajalla. Saran-saran dan pendapat yang membangun dari pembaca akan sangat membantu bagi perbaikan buku ini. Penulisan buku ini juga telah melalui review buku oleh Dr. Iwan Sugihartono (Fisika FMIPA UNJ). Untuk itu kami ucapkan terima kasih bagi semua pihak yang memberikan kontribusi untuk terwujudnya buku ini.

Jember, Kampus Tegal Boto, November 2022

Penulis **AMZ**

KATA PENGANTAR PAKAR SEBIDANG ILMU

Pertama kali saya mengucapkan selamat kepada penulis (AMZ) yang sudah berhasil menyelesaikan buku "Metode Simulasi Dinamika Molekul dan Aplikasinya".

Buku ini merupakan buku yang sangat berguna bagi siapa saja yang tertarik pada bidang komputasi, khususnya mahasiswa tingkat akhir yang sedang melakukan riset tugas akhir bidang Komputasi Fisika *Condensed Matter* dan bagi mahasiswa yang sedang mempelajari aplikasi komputasi Fisika. Sesuai dengan judulnya maka dengan mempelajari buku ini pembaca diharapkan dapat memprediksi/menghitung besaran-besaran dinamik sistem materi yang berkaitan dengan gerak molekul-molekulnya seperti koefisien difusi, tegangan permukaan, entalpi, volume, temperatur, energi total dan sebagainya menggunakan program komputer LAMMPS dan MOLDY dengan dukungan software-software pendukung seperti Packmol, OVITO dan sebagainya.

Di dalam buku ini, penulis secara sistematis menjelaskan bagaimana program komputer LAMMPS dan MOLDY di *install* ke dalam sistem operasi *linux*. Namun demikian, sistem operasi windows juga dapat digunakan. Salah satu kelebihan buku ini adalah program-program komputer dan sistem operasi linux yang digunakan semua tersedia di internet. Para pembaca yang ingin mempelajari dan mencoba melakukan simulasi menggunakan program dan sistem operasi tersebut tidak perlu kuatir mengeluarkan biaya. Metode dinamika molekul juga disuguhkan oleh penulis secara komprehensif disertai dengan prosedur simulasi yang terstruktur. Penulis juga memandu pembaca dengan menyuguhkan pula contoh pemrograman sederhana dinamika molekul menggunakan bahasa pemprograman C++. Sedangkan di bagian akhir buku ini, penulis memberikan ide bagaimana menemukan suatu ide melakukan riset dinamika molekul menggunakan program Moldy dan LAMMPS dan dukungan program Packmol, Ovito. Penulis telah menambahkan beberapa bagian materi yang sangat penting misalnya pada penggunaan program Atomsk dan juga website-website penting.

Menurut pendapat saya, buku ini dapat memberikan inspirasi dan manfaat dalam menunjang riset dibidang Fisika *Condensed Matter* berbasiskan komputasi. Akhir kata, saya mengucapkan terima kasih sudah diberi kesempatan untuk membaca dan menelaah buku ini, dan semoga buku ini dapat memberikan wawasan, khazanah baru, dan inspirasi bagi mahasiswa atau siapa saja yang sedang menekuni riset Fisika khususnya bidang *Condensed Matter*, Ilmu Material, dan bidang terapan Fisika komputasi.

Jakarta, Oktober 2022

Dr. Iwan Sugihartono, MSc.
Grup Fisika Semikonduktor dan Nano-Struktur
Jurusan Fisika FMIPA Universitas Negeri Jakarta

DAFTAR ISI

DAFTAR GAMBAR

DAFTAR TABEL

KRONOLOGI METODE DINAMIKA MOLEKUL

1900	Konsep medan gaya dalam analisis spektroskopi
1929	Potensial atom (Morse dan Lennard-Jones)
1937	Dispersi London
1946	Mekanika Molekuler
1953	Simulasi Monte Carlo
1957	Simulasi Dinamika Molekul Hard Sphere (Alder dan Wainwright)
1964	Simulasi Dinamika Molekul Gas Argon potensial Lennard-Jones (A Rahman)
1967	Algoritma Verlet oleh Loup Verlet
1970	Simulasi Liquid. Pengembangan potensial Born-Mayer-Huggins, BMH)
1976	Simulasi SiO_2 (silica) dengan potensial BMH
1980	Algoritma Anderson Constant-Pressure
	Algoritma Rahman Parrinello Constant-Pressure
1985	Metode Dinamika Molekul Kuantum Car-Parrinello (CPMD) dengan DFT
1990	Potensial Interaksi Stillinger-Weber
2000 -	Software Dinamika Molekul Paralel: MOLDY, NAMD, OVITO, LAMMPS, PACKMOL, ATOMSK dan lain-lain

LAMPIRAN

L1. Hasil Riset di Annals of Nuclear Energy

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Inhibition of iron corrosion in high temperature stagnant liquid lead: A molecular dynamics study

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ABSTRACT

Corrosion property of iron in high temperature stagnant liquid lead has been studied using molecular dynamics method. The method was used to predict the limit values of the injected oxygen into the liquid lead for maximum corrosion inhibition of iron. It is from experimental results, in order to inhibit the corrosion at possible lowest rate then a stable self-healing protective iron oxide layer should be developed at the surface of steel continuously. In this research we investigated the iron corrosion and it can be predicted that the protective oxide layer may be formed by injecting oxygen within the range of 5.35×10^{-2} wt% to 8.95×10^{-2} wt% (for observed temperature 750 °C). The oxygen 5.35×10^{-2} wt% is the lower limit to prevent high dissolution of iron while the oxygen content of 8.95×10^{-2} wt% is the upper limit to avoid high precipitation of lead oxide. We also guess that effect of oxygen injection into liquid lead creates a thin oxygen barrier that separating the liquid lead and iron oxides from direct interaction. The iron oxides layer and oxygen barrier then may be regarded as double corrosion inhibition.

1. Introduction

For design of fast nuclear reactors, lead (Pb) is one of popular coolant material candidates (Zhang and Li, 2008). Liquid lead has boiling temperature 1740 °C which is above the melting temperature of reactor clad, and also has relatively low melting point 327 °C (Bentor and Yinon, 2013). Lead is also chemically inert with respect to water compared with the sodium. Lead has also high thermal conductivity compared with water. Those physical and chemical properties determine margins of its operation region in reactor application (Sobolev, 2007). However, it is well known that the cladding and structural materials are severely corroded if they are exposed to high temperature liquid lead directly. The dissolution of steel components under high temperature liquid lead is very high (Kashezhev et al., 2010; Zelenskii et al., 2007; Zhang et al., 2010; Zhang and Li, 2008). High dissolution of iron in liquid lead causes destruction (corrosion) of iron (Manly, 1959). The corrosion exactly has limited the lifetime of reactor operation, and this crucial problem has presented a critical challenge in application of liquid lead for design of fast reactor. We need to know a way for inhibiting strong corrosion of liquid lead or developing corrosion-resistant novel materials, not only under normal condition but also in temporary anomalous condition (Rivai and Takahashi, 2010).

Although many experiments about liquid lead/lead alloys corrosion have been reported, however a fully understanding how to manage the corrosion are still not completed, yet. In addition, not all experiments may or easy be done within an operating reactor. In this situation then simulation methods have become a promising technique for studying corrosion. However, the number of publications about simulation of corrosion phenomena of liquid lead is still few, especially using molecular dynamics (MD) simulation method. Maulana et al. (2008) in their preliminary work had studied the penetration depth of atoms of liquid lead into Fe–Ni–Cr steel by using the Lennard-Jones (LJ) MD simulation. However they did not explore the thermodynamics properties of the corrosion such as the diffusion coefficient and also did not study the corrosion inhibition mechanism. In the previous work (Arkundato et al., 2010) we had applied the MD simulation method to calculate the diffusion coefficient of iron in stagnant liquid lead. In the current work we study corrosion inhibition. To realize the simulations we used the MOLDY MD program that is a powerful technique for material computation (Ackland et al., 2011; Refson, 2000).

A technique of reducing the corrosion is to develop a stable self-healing protective oxide layers on the surface of structural materials (cladding, pipe, vessel system, etc.) to prevent direct high dissolution of metal components. This protective layer may be developed by maintaining the dissolved oxygen into liquid lead (Bolind, 2009; Rivai and Takahashi, 2010; Zelenskii et al., 2007; Zhang et al., 2010; Zhang and Li, 2008). This protective oxide layers cut down the dissolution rate of material components of the

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L2. Hasil Riset di Turkish Journal of Physics

TÜBİTAK

Turkish Journal of Physics

http://journals.tubitak.gov.tr/physics/

Research Article

Turk J Phys
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Molecular dynamic simulation on iron corrosion-reduction in high temperature molten lead-bismuth eutectic

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Abstract: Molecular dynamic simulation on iron in high-temperature molten lead-bismuth eutectic has been carried out to investigate the iron corrosion and its mitigation. The aim of the work is to investigate the corrosion and evaluate proper oxygen content of injection for significant and effective reduction. To study the phenomena we calculated the diffusion coefficients, radial distribution functions and mean square displacement of iron, and also observed the microstructure of iron before and after oxygen injection into coolant. The present calculation shows that a significant and effective reduction of corrosion can be achieved by injection of 7.68×10^{-2}–1.55×10^{-1} wt% into coolant at temperature 750 °C. It is predicted that the lower limit of oxygen content, 7.68×10^{-2} wt%, is the minimum value to develop a self-healing stable protective oxide film for preventing high dissolution of iron; and that the upper limit of oxygen content, 1.55×10^{-1} wt%, is the maximum value in order to avoid the precipitation of coolant oxides. By injection of 7.68×10^{-2} wt% of oxygen, the corrosion rate has been reduced about 92.16% at 750 °C, and reduced by 98.66% at the lower temperature 550 °C, compared with the normal, oxygenless condition.

Key words: Corrosion of pure iron, lead-bismuth eutectic, molecular dynamic, diffusion, oxygen content

1. Introduction

It has been known that the lead-bismuth eutectic (LBE) is an important coolant candidate for advanced nuclear-reactors design. This coolant has advantage properties such as low melting temperature (∼125.1 °C), high boiling temperature (∼1670 °C) and chemical stability [1–3]. However, it is also well known that the fuel cladding of the reactor is severely corroded due to its interaction with high temperature molten LBE [3–6]. The LBE has high solubility for iron, chromium and especially nickel at high temperatures. Since solubility is temperature dependent, the LBE tends to dissolve the structural materials (cladding) in the hot sections of the system and precipitate it in the cold sections of the system, clogging the piping [7]. This problem has brought critical challenges, i.e. how to reduce the corrosion rate and/or how to design novel corrosion-resistant materials. The corrosion process must be understood, controlled and reduced for safety and economic reasons.

One technique to reduce the corrosion is to develop a stable oxide scale (self-healing protective films) on the structural materials (cladding, pipe, vessel system, etc.) surfaces to prevent direct dissolution of metal components by maintaining the necessary concentration of dissolved oxygen in the LBE coolant [5, 7–11]. This protective oxide reduces the dissolution of structural materials into LBE, since the material components

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L3. Hasil Riset di Journal of Physics: Conference Series

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Molecular dynamics simulation of corrosion mitigation of iron in lead-bismuth eutectic using nitrogen as corrosion inhibitor

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Abstract. The corrosion of structural materials used in fast nuclear reactor design is a current major problem. It is due to the use of liquid metal as a coolant candidate in the heat transfer system. The liquid metal as lead-bismuth eutectic was found to make high corrosion to structural material as steel. One of the solutions of this problem is to inject some inhibitor into liquid metal. In this current work we simulate the effect of nitrogen injection as inhibitor candidate. The simulation will predict the proper concentration of injected nitrogen and also observe the microscopic structure of the material before and after injection to know the ability of nitrogen as an inhibitor. The simulation follows the molecular dynamics method and for preliminary study we use iron material rather than steel. We also use lennard-jones potential for simplification of the study. It is from our simulation we see nitrogen shows better corrosion mitigation compare with oxygen as in our previous study. The effective inhibition can be achieved by injecting at least 0.056wt.% nitrogen. This amount seems to be able to reduce the corrosion level of iron till about 99.5% for high corrosion at temperature 750 °C.

Keyword: lead-bismuth eutectic, corrosion inhibition, nitrogen, molecular dynamics

1. Introduction

Corrosion inhibitor is a substance which when added in small concentration to a corroded system will minimize or prevents that corrosion [1]. Corrosion inhibitor can be used to protect metals from corrosion attach and if we can maintain this inhibitor in an exact concentration all the time than we will be able to prevent the corrosion maximally. It is a current issue that the steels used in the fast nuclear reactor installation have been highly corroded if we use liquid lead or lead bismuth eutectic as a coolant material for heat transfer system [2]. The solution of this corrosion problem has two options: (1) finding better steel materials and/or (2) finding a corrosion inhibitor (method) to minimize and

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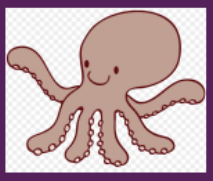
L4. Parameter Potensial Lennard-Jones

TABLE

LJ Potential parameters of atoms and other related properties



Dr. Artoto Arkundato V01.07July2022

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[6] phys. stat. sol. (a) 78, 595 (1983)

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[9] doi:10.3906/fiz-1112-12

[10] Molecular Simulation, Vol. 30 (4), 15 April 2004, pp. 205–216

Atomic number	Atom	Mol Weight u	Density gr/cm^3	Melting (K)	Crystal structure	Lattice const. (A)	Epsilon (eV)	Sigma (A)	Thermal con W/(m K)
1	**H**	1.0080 [1]	0.000089 [1]	13.81 [1]	gas		0.002516 [7]	2.87 [7]	0.1805 [2]
2	He	4.0026 [1]	0.000179 [1]	0.95K [1]	gas		0.000939 [8]	2.64 [8]	0.1513 [2]
3	Li	7.0 [2]	0.534 [2]	453.65 [2]	BCC	351 pm [3]	0.199543 [6]	2.8517 [6]	85 [3]
4	Be	9.01218 [2]	1.85 [2]	1560 [2]	simple hex	228.58, 228.58,pm 358.43 [3]			190 [3]
5	B	10.81 [3]	2.46 [3]	2348 [3]	simple tri	506 pm [3]			27 [3]
6	C	12.011 [3]	2.26 [3]	3823 [3]	simple hex	246.4, 246.4 pm, 671.1 [3]	0.4396 kJ/mol [10]	3.4309 [10]	140 [3]
7	N	14.007 [2]	1.251 g/l [2]	62.9 [2]	gas		0.00819[7]	3.7 [7]	0.0258 [2]
8	O	15.999 [2]	1.429 g/l [2]	54.7 [2]	gas		0.010167[7]	3.46 [7]	0.0266 [2]
10	Ne	20.1797 [2]	0.9 g/l[2]	24.41 [2]	gas		0.0030 [7]	2.78 [7]	140 [2]
11	Na	22.9898 [2]	0.968 [2]	97.72	BCC [6]	4.2906 pm [2]	0.136007 [6]	3.4276 [6]	
12	Mg	24.305 [2]	1.738	923 [2]	BCC [6]	320.94, 320.94, 521.08 pm [2]	0.178499 [6]	2.9234 [6]	160 [2]
13	Al	26.9815[2]	1.251 g/l [2]	933.32	FCC [4]	4.0495 pm [2]	0.0435 [4]	2.5735 [4]	235 [2]
14	Si	28.085 [2]	2.33 [2]	1687 [2]	FCC [4]	543.09 pm [2]	0.0594 [4]	2.5735 [4]	235 [2]
15	P	30.97376 [2]	1.823 [2]	317.2 [2]	FCC [4]	simple triclinic 1145, 550.3, 1126.1 pm [2]	0.0191 [4]	3.6564 [4]	0.235 [2]
18	Ar	39.948 [2]	1.784 [2]	83.7 [2]	gas		0.0105 [7]	3.4 [7]	
22	Ti	47.867 [2]	4.507 [2]	1942 [2]	HCP[4]	simple hexa 295.08, 295.08, 468.55 pm	0.0330 [4]	2.6843 [4]	22 [2]
23	V	50.9415 [2]	6.11 [2]	2183 [2]	BCC[4]	303 pm [2]	0.0084 [4]	2.4390 [4]	31 [2]
24	Cr	51.9961 [2]	7.19 [2]	1907 [2]	BCC[4]	291 pm [2]	0.0160 [4]	2.2811 [4]	
	Cr				BCC[5]	2.884 [5]	0.6732 [5]	2.2813 [5]	94 [2]
25	Mn	54.93804 [2]	7.47 [2]	1519 [2]	BCC[4]	891.25 pm [2]	0.0091 [4]	2.3187 [4]	7.7 [2]
26	Fe				FCC[4]		0.1584 [4]	2.3193 [4]	79 [2]
	α-Fe	55.845 [2]	7.874 [2]	1811 [2]	BCC[5]	2.8664 [5]	0.7064 [5]	2.2674 [5]	79 [2]
27	Co	58.933194 [2]	8.9 [2]	1768 [2]	HCP[4]	simple hexa 250.71, 250.71, 406.95 pm [2]	0.0172 [4]	2.2805 [4]	
	Co				HCP[6]		0.51582 [6]	2.284 [6]	100 [2]
28	Ni	58.6934 [2]	8.908 [2]	1728 [2]	FCC[4]		0.0174 [4]	2.2805 [4]	91 [2]
	Ni				FCC[6]	3.5238 [5]	0.6609 [5]	2.2395 [5]	
	Ni				FCC[6]	352.4 pm [2]	0.519 [6]	2.2808 [6]	

29	Cu	63.546 [2]	8.96 [2]	1357.6 [2]	FCC[4]	361.49 pm [2]	0.0124 [4]	2.2966 [4]	400 [2]
34	Se	78.971 [2]	4.819 [2]	494 [2]	HCP[4]	simple monoclinic 905.4, 908.3, 1160.1 pm [2]	0.1601 [4]	3.1888 [4]	0.52 [2]
35	Br				HCP[4]		0.0745 [4]	2.5736 [4]	0.12 [2]
40	Zr	91.224 [2]	279.511 [2]	2128 [2]	HCP[4]	simple hexa 323.2, 323.2, 514.7 pm	0.0126 [4]	2.9314 [4]	23 [2]
41	Nb	92.90637 [2]	8.57 [2]	2750 [2]	BCC[4]	330.04 pm [2]	0.0522 [4]	2.6818 [4]	54 [2]
42	Mo	95.95 [2]	10.28 [2]	2896 [2]	BCC[4]	314.7 pm [2]	0.1510 [4]	2.4892 [4]	
	Mo				BCC[5]	3.1468	1.112 [5]	2.4892 [5]	139 [2]
59	Ta	180.94788 [2]	16.65 [2]	3290 [2]	BCC[4]	330.13 pm [2]	0.0558[4]	2.682 [4]	57[2]
60	W	183.84 [2]	19.25 [2]	3695 [2]	BCC[4]	316.52 pm [2]	0.1227 [4]	2.5619 [4]	170 [2]
64	Pt	195.084 [2]	21.45 [2]	2041.3 [2]	FCC[6]	392.42 pm [2]	0.68152[6]	2.5394 [6]	71 [2]
65	Au	196.9665 [2]	19.3 [2]	337.18 [2]	FCC[6]	407.82 pm [2]	0.44404[6]	2.6367 [6]	320 [2]
68	Pb	207.2 [2]	11.34 [2]	500.46 [2]	FCC[4]	495.08 pm [2]	0.265 [4]	3.189 [4]	35 [2]
69	Bi	208.9804 [2]	9.78 [2]	544.3 [2]		Base-centered Monoclinic 667.4, 611.7, 330.4 pm [2]	0.059 [9]	3.05 [9]	8 [2]

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

r is the distance between two interacting particles
ε is the depth of the potential well (dispersion energy)
σ is the distance at which energy V is zero ('size of the particle')

L5. Parameter Potensial Morse

TABLE

Morse Potential param. of atoms and other related properties

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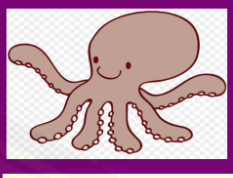

Dr. Artoto Arkundato
Ver.23July2022

Atomic number	Atom	Mol Weight u	Density gr/cm^3	Melting (K)	Crystal structure	Lattice const. (A)	D (eV)	alpha (Å^-1)	r (Å)	Thermal C. W/(m K)
1	**H_2**	1.0080 [1]	0.0000899 [1]	13.81 [1]	gas		0.00046 [10]	1.923 [10]	3.29 [10]	0.1805 [2]
2	He	4.0026 [1]	0.0001785 [1]	0.95K [1]	gas		0.0001 [10]	2.197 [10]	2.92 [10]	0.1513 [2]
3	Li	7.0 [2]	0.534 [2]	453.65 [2]	BCC	351 pm [3]	0.0228 [7]	0.4441 [7]	7.461 [7]	85 [3]
4	Be	9.01218 [2]	1.85 [2]	1560 [2]	simple hex	228.58, 228.58,pm 358.43 [3]				190 [3]
5	B	10.81 [3]	2.46 [3]	2348 [3]	simple trig	506 pm [3]				27 [3]
6	C	12.011 [3]	2.26 [3]	3823 [3]	simple hex	246.4, 246.4 pm, 671.1 [3]	2.423 [11]	2.555 [11]	2.522 [11]	140 [3]
	C						0.93810[13]	1.43160[13]	1.9014 [13]	
7	N_2	14.007 [2]	1.251 g/l [2]	62.9 [2]	gas		0.00682 [10]	1.166 [10]	4.43 [10]	0.0258 [2]
	N						4.44 [11]	2.096 [11]	1.35 [11]	
8	O_2	15.999 [2]	1.429 g/l [2]	54.7 [2]	gas		0.01119 [10]	1.1542 [10]	3.75 [10]	0.0266 [2]
	O						0.042117 [12]	1.1861 [12]	3.70366 [12]	
10	Ne	20.1797 [2]	0.9 g/l[2]	24.41 [2]	gas		0.0027 [10]	2.036 [10]	3.09 [10]	140 [2]
11	Na	22.98977 [2]	0.968 [2]	97.72	BCC	4.2906 pm [2]	0.0633 [8]	0.3899 [8]	5.336 [8]	
	Na						0.0314 [7]	0.5847 [7]	5.65 [7]	
12	Mg	24.305 [2]	1.738	923 [2]	BCC	320.94, 320.94, 521.08 pm [2]	0.5404 [17]	0.7921 [17]	3.1814 [17]	160 [2]
13	Al	26.9815[2]	1.251 g/l [2]	933.32	FCC	4.0495 pm [2]	0.2703 [8]	1.1646 [8]	3.253 [8]	235 [2]
	Al						0.2700[9]	1.0341 [9]	3.4068 [9]	
14	Si	28.085 [2]	2.33 [2]	1687 [2]	FCC	543.09 pm [2]	0.9862 [5]	1.3642 [5]	2.8429 [5]	235 [2]
	Si					simple	0.227 [11]	4.499 [11]	1.54 [11]	
15	P	30.97376 [2]	1.823 [2]	317.2 [2]	FCC	triclinic 1145, 550.3, 1126.1 pm [2]				0.235 [2]
18	Ar	39.948 [2]	1.784 [2]	83.7 [2]	gas		0.00893 [10]	1.253 [10]	4.13 [10]	
19	K	39.0983 [2]	0.856 [2]	336.34[2]	BCC [2]	532.8, 532.8, 532.8 pm [2]	0.0542 [8]	0.4976 [8]	6.369 [8]	100 [2]
	K						0.0285 [7]	0.4958 [7]	6.758 [7]	
20	Ca	40.078 [2]	1.55 [2]	1115 [2]	FCC [2]	558.84, 558.84, 558.84 pm [2]	0.1623 [8]	0.8053 [8]	4.569 [8]	200 [2]
22	Ti	47.867 [2]	4.507 [2]	1942 [2]	HCP	simple hexa 295.08, 295.08, 468.55 pm	1.02795 [12]	3.64074 [12]	1.88265 [12]	22 [2]
23	V	50.9415 [2]	6.11 [2]	2183 [2]	BCC	303 pm [2]	0.2552 [7]	1.1919 [7]	3.234 [7]	31 [2]

24	Cr	51.9961 [2]	7.19 [2]	1907 [2]	BCC	291 pm [2]	0.4414 [8]	1.5721 [8]	2.754 [8]	
	Cr				BCC	2.884 [5]	0.2372 [7]	1.4709 [7]	2.909 [7]	94 [2]
25	Mn	54.93804 [2]	7.47 [2]	1519 [2]	BCC	891.25 pm [2]				7.7 [2]
26	Fe BCC				FCC		0.4174 [8]	1.3885 [8]	2.845 [8]	79 [2]
	Fe BCC	55.845 [2]	7.874 [2]	1811 [2]	BCC	2.8664 [5]	0.2192 [7]	1.324 [7]	2.998 [7]	79 [2]
	Fe BCC						0.418 [6]	1.397 [6]	2.849 [6]	
	Fe						0.42 [18]	1.40 [18]	2.85 [18]	
	Fe						0.1309 [19]	2.412 [19]	2.56 [19]	
27	Co	58.933194 [2]	8.9 [2]	1768 [2]	HCP	simple hexa 250.71, 250.71, 406.95 pm [2]	0.42 [16]	1.38 [16]	2.8 [16]	100 [2]
	Co						0.5827 [19]	2.052 [19]	2.37 [19]	
28	Ni	58.6934 [2]	8.908 [2]	1728 [2]	FCC	3.5238 [5]	0.4205 [8]	1.4199 [8]	2.78 [8]	91 [2]
	Ni				FCC	352.4 pm [2]				
29	Cu	63.546 [2]	8.96 [2]	1357.62 [2]	FCC	361.49 pm [2]	0.3429 [8]	1.3588 [8]	2.866 [8]	400 [2]
	Cu						0.3282 [9]	1.3123 [9]	2.8985 [9]	
	Cu						0.3429 [16]	1.3588 [16]	2.866 [16]	
32	Ge	2.63 [2]	5.323 [2]	1211.3 [2]	FCC [2]	565.75, 565.75, 565.75 pm [2]	0.9675 [5]	1.5569 [5]	2.8319 [5]	60 [2]
34	Se	78.971 [2]	4.819 [2]	494 [2]	HCP	simple monoclinic 905.4, 908.3, 1160.1 pm [2]				0.52 [2]
38	Sr	87.62 [2]	2.63 [2]	1050 [2]	FCC [2]	608.49, 608.49, 608.49 pm [2]	0.1513 [8]	0.7377 [8]	4.988 [8]	35 [2]
40	Zr	91.224 [2]	279.511 [2]	2128 [2]	HCP	simple hexa 323.2, 323.2, 514.7 pm	0.858 [15]	1.5 [15]	3.09 [15]	23 [2]
40	Zr	91.42 [15]			BCC [15]	3.62 A [15]	0.858 [15]	1.5 [15]	3.09 [15]	23 [2]
41	Nb	92.90637 [2]	8.57 [2]	2750 [2]	BCC	330.04 pm [2]	0.3501 [7]	1.0705 [7]	3.556 [7]	54 [2]
42	Mo	95.95 [2]	10.28 [2]	2896 [2]	BCC	314.7 pm [2]	0.8051 [6]	1.5102 [6]	3.012 [6]	
	Mo				BCC	3.1468	0.8032 [8]	1.5079 [8]	2.976 [8]	139 [2]
47	Ag	107.8682 [2]	10.49 [2]	1234.78 [2]	FCC[2]	408.53, 408.53, 408.53 pm [2]	0.3323 [8]	1.369 [8]	3.115 [8]	430 [2]
	Ag						0.3253 [9]	1.3535 [9]	3.13 [9]	
	Ag						0.3638 [19]	1.669 [19]	2.92 [19]	
55	Cs	132.905 [2]	1.879 [2]	301.44 [2]	BCC[2]	614.1, 614.1, 614.1 pm [2]	0.0448 [8]	0.4156 [8]	7.557 [8]	36[2]
	Cs						0.0276 [7]	0.4552 [7]	7.505 [7]	
59	Ta	180.94788 [2]	16.65 [2]	3290 [2]	BCC	330.13 pm [2]	0.786 [8]	1.573 [8]	3.326 [8]	57[2]
							0.4041 [7]	1.1257 [7]	3.485 [7]	
60	W	183.84 [2]	19.25 [2]	3695 [2]	BCC	316.52 pm [2]	0.9906 [8]	1.4116 [8]	3.032 [8]	170 [2]
							0.5157 [7]	1.3857 [7]	3.152 [7]	
	W						0.9906 [6]	1.441 [6]	3.042 [6]	
64	Pt	195.084 [2]	21.45 [2]	2041.3 [2]	FCC	392.42 pm [2]	0.6744 [19]	1.817 [19]	2.79 [19]	71 [2]
65	Au	196.9665 [2]	19.3 [2]	337.18 [2]	FCC	407.82 pm [2]	0.4753 [9]	1.583 [9]	3.0242 [9]	320 [2]
	Au						0.4341 [19]	1.797 [19]	2.90 [19]	
68	Pb	207.2 [2]	11.34 [2]	500.46 [2]	FCC	495.08 pm [2]	0.2348 [8]	1.1836 [8]	3.733 [8]	35 [2]
	Pb						0.2027 [19]	1.563 [19]	3.42 [19]	
69	Bi	208.9804 [2]	9.78 [2]	544.3 [2]		Base-centered Monoclinic 667.4, 611.7, 330.4 pm [2]	0.085 [14]	2.212 [14]	4.203 [14]	8 [2]

$$\varepsilon(r_{ij}) = D\left\{e^{-2\alpha(r_{ij}-r_o)} - 2e^{-\alpha(r_{ij}-r_o)}\right\}$$

ε(rij)	atomic potential of two atom separated by rij
D (eV)	dept of potential well; dissociation energy
alpha (1/A)	inverse of width of well; bond rigidity

INDEKS

BIOGRAFI PENULIS

(A) Dr. Artoto Arkundato lahir di Srengat, Blitar, Jawa Timur, pada 25 Desember 1969. Sekolah SD, SMP dan SMA diselesaikan di Blitar, tepatnya di SMAN 1 Blitar. Kemudian melanjutkan kuliah pada Jurusan Fisika, FMIPA, UGM di Yogyakarta. Lulus kuliah S1 dengan menyelesaikan skripsi teori yang berjudul Aspek Klasik dan Kuantum Optika Nonlinear dengan pembimbing Prof. Muslim, Phd dan Dra. Zahara, MSc. Setelah lulus kuliah sempat bekerja di dunia Industri di beberapa *multinational company* seperti SINOCA (Eks AT&T), Quantum Matshushita ltd. dan Symens Component Electronics di BATAM. Pada 1999 memutuskan untuk kembali ke dunia pendidikan yaitu mengabdi di Jurusan Fisika FMIPA Universitas Jember. Kuliah lanjut S2 diselesaikan di Jurusan Fisika FMIPA ITB pada 2003 dengan mengambil thesis mengenai metode komputasi Bruckner Hartree-Fock untuk aplikasi problem hamburan nuklir dengan Pembimbing Utama Prof. Zaki Su'ud,. Kuliah S3 juga diselesaikan di Jurusan Fisika FMIPA ITB Bandung pada 2012 mengambil topik disertasi aplikasi metode simulasi dinamika molekul untuk mengamati proses dan penghambatan korosi logam cair dalam reaktor nuklir, dengan promotor utama Prof. Zaki Su'ud, Co-promotor Prof. Mikrajudin Abdullah dan Dr. Widayani.

Pelatihan metode komputasi yang pernah diikuti adalah *Workshop on Material Computation* di JNCASR, Bangalore, India pada 2005 yang diselenggarakan ICTP Italia. Kegiatan *visiting researcher* yang pernah diikuti adalah ke ENEA Roma, Italia pada 2010 untuk memperdalam metode simulasi dinamika molekul paralel menggunakan ENEA grid supercomputing dengan supervisor Dr. Massimo Celino. Pada 2018 mengunjungi Osaka University pada Lab Theoretical NanoTechnology dengan Ptof. Tamio Oguchi sebagai supervisor. Artoto Arkundato mengajar beberapa matakuliah seperti Fisika Kuantum, Fisika Inti, Komputasi Atom dan Molekul serta Fisika Komputasi.

(M) Dr. Moh. Hasan lahir di Malang, 04 April 1964 adalah dosen Jurusan Matematika pada FMIPA Universitas Jember. Aktif mengajar dengan beberapa matakuliah yang pernah dibina seperti Pemodelan Matematika, Komputasi Matriks, Analisa Numerik dan Sistem Dinamik. Dr. Moh. Hasan memperoleh pendidikan doktor dari Wageningen University, Belanda.

(Z) Prof. Zaki Suud adalah dosen aktif Jurusan Fisika FMIPA ITB Bandung. Menyelesaiakan S1 pada Jurusan Fisika FMIPA ITB Bandung pada 1986. Studi lanjut S2 pada Magister Engineering, Dept. of Nuclear Engineering, Tokyo Inst. of Technology (1992 sedangkan Studi lanjut S3 pada Dept. of Nuclear Engineering, Tokyo Institute of Technology (TIT) Jepang yang diselesaikan pada 1995. Beberapa matakuliah penting yang pernah berikan adalah Fisika Reaktor, Komputasi Nuklir, Fisika Inti, dan Mekanika Kuantum. Prof. Zaki Suud aktif meneliti desain reaktor nuklir dan merupakan salah satu pakar fisika reaktor di Indonesia serta telah membimbing serta meluluskan banyak mahasiswa doktoral di Fisika FMIPA ITB.

RINGKASAN BUKU

Untuk melaksanakan riset material secara teoretik maka ada banyak metode yang dapat dipilih dan dilakukan. Salah satunya yang sangat handal adalah metode simulasi dinamika molekul. Metode ini sebenarnya adalah berusaha mempelajari dan mengkaji fenomena alam mikroskopis dengan cara atau menggunakan pendekatan makroskopis yaitu menggunakan hukum gerak Newton. Oleh karena kompleksitas fenomena alam dan juga jumlah partikel yang diteliti yang mungkin saja perlu dalam jumlah besar maka persamaan gerak ini menuntut dikerjakan dalam perangkat komputer dan oleh karena itu dalam bentuk program komputer. Beberapa pendekatan untuk menyelesaikan persamaan gerak Newton secara numerik ada dalam metode ini. Berbagai program simulasi dinamika molekul (MD) juga telah banyak dibuat baik yang boleh digunakan secara gratis maupun harus membeli untuk mendapatkan lisensinya. Pada buku ini digunakan program-program yang gratis dan/atau open-source seperti MOLDY, LAMMPS, OVITO, PACKMOL, ISSACS dan ATOMSK.

Buku ini disusun sedemikian hingga pembaca yang tertarik riset metode simulasi dinamika molekul dapat belajar dari awal, membuat yang sederhana sampai hanya menggunakan software-software yang sudah ada. Buku ini disiapkan agar pembaca dapat memulai melakukan riset atau penelitian dalam bidang fisika material meskipun juga pada kenyataanya metode simulas MD ini dapat diterapkan dan dikembangkan ke banyak sekali bidang kajian seperti Biologi, Kimia, Farmasi, Astrofisika, Geofisika, Biofisika bahkan ke ekonofisika.

Simulasi dinamika molekul menawarkan peluang untuk menemukan material unggul yang dapat dimanfaatkan untuk berbagai keperluan dan aplikasi. Terakhir penulis mempunyai harapan agar riset dalam bidang aplikasi dinamika molekul ini dapat berkembang dengan baik ke depan, dapat bersinergi dengan riset terapan untuk dapat menghasilkan karya-karya dan produk-produk yang berguna bagi bangsa Indonesia.

Buku ini sebagian besar memberikan materi untuk keperliuan riset dan juga memaparkan hasil-hasil penelitian khususnya menggunakan software MOLDY, Ovito dan Atomsk.