



DAFTAR PUSTAKA

- Aller, L., Howerd, A., Hassard, J., dan Mainwood, A., 1997, Neutron damage of CVD diamond, *Diamond Relat. Mater.* 6, 353.
- Al-Mushadani, O. dan Needs, R., 2003, Free-energy calculations of intrinsic point defects in silicon, *Phys. Rev. B* 68, 235205.
- Austin, I. dan Wolfe, R., 1956, and Optical Properties of a Semiconducting Diamond, *Proc. Phys. Soc. B* 69 329.
- Baima, J., Zelferino, A., Olivero, P., Erba, A., dan Dovesi, R., 1961, Raman spectroscopic features of the neutral vacancy in diamond from ab initio quantum-mechanical calculations ,*Phys Chem Chem Phys* 18(3).
- Battiato, A., Lorruso, M., Bernardi, E., Picollo, F., Bosia, F., Uguen, D., Zelferino, A., Darmin, A., Baima, J., Pugno, N., Ambrisio, E., dan Olivero, p., 2016, Softening the ultra-stiff: Controlled variation of Young's modulus in single-crystal diamond by ion implantation, *Acta Materialia* 116, 95-103.
- Berman, R. 1992, *In The Properties of Natural and Synthetic Diamond*, edited by J. E. Field, Academic Press, London.
- Bernholc, J., Antonelli, A., dan Sole, T., 1988, Mechanism of Self-Diffusion in Diamond, *Phys. Rev. Lett.* 61, 2689.
- Birch, F., 1947, Finite Elastic Strain of Cubic Crystals, *Phys. Rev.* 71, 809.
- Boas, M., 1983, *Mathematical Methods in The Physical Sciences*, John Wiley Sons, New York.
- Bourgoin, J., 1983, An experimental estimation of the vacancy formation energy in diamond,*Radiation Effects*, 79:1-4, 235-239.
- Burton, J., 1972, Vacancy-Formation Entropy in Cubic Metals, *Phys. Rev. B* 5, 2948.
- Chang, K dan Cohen, M., 1987, Understanding the thermal conductivity of Diamond/Copper composites by first-principles calculations, *Carbon* 148 249-257.



- Chang, S., Barnard, A., Dwyer, C., Boothroyd, C., Hocking, R., Osawa, E., dan Nicholls, R., 2016, Counting vacancies and nitrogen-vacancy centers in detonation nanodiamond, *Nanoscale*, 2016, 8, 10548-10552 .
- Chen, L., Chen, S., dan Hou, Y., 2019, Ab initio pseudopotential study of structural and high-pressure properties of SiC, *Phys. Rev. B* 35, 8196.
- Corsetti, F. dan Mostofi, A., 2011 , System-size convergence of point defect properties: The case of the silicon vacancy, *Phys. Rev. B* 84, 035209.
- Dannefaer, S., Mascher, P., dan Kerr, D., 1986, Monovacancy Formation Enthalpy in Silicon, *Phys. Rev. Lett.* 56, 2195.
- Davies, G. dan Nazare,M. , 1980, Uniaxial stress splitting of E to E transitions at trigonal centres in cubic crystals: the 594 nm band in diamond, *J. Phys. C* 13, 4127.
- Edwards, D. dan Ochoa, E., 1981, Infrared refractive index of diamond, *J. Opt. Soc. Am.* 71, 607-608.
- Glensk, A., Grabowski, B., Hickel, T., dan Neugebauer, J., 2014, Breakdown of the Arrhenius Law in Describing Vacancy Formation Energies: The Importance of Local Anharmonicity Revealed by Ab initio Thermodynamics, *Phys. Rev. X* 4, 011018.
- Hadlington, S., 2005, single crystal diamond for power semiconductor devices, *IEE Review* 51, 30.
- Hartree, D., 1928, The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part I. Theory and Methods, *Mathematical Proceedings of the Cambridge Philosophical Society*, 24, 89-110.
- Hehenkamp T., 1994, Absolute vacancy concentrations in noble metals and some of their alloys, *J. Phys. Chem. Solids* Vol. 55, No. 10, pp. 907-915.
- Hohenberg, P. dan Kohn, W., 1964, Inhomogeneous Electron Gas, *Phys. Rev.* 136, B864.
- Hood, R., 2003, Quantum Monte Carlo Study of the Optical and Diffusive Properties of the Vacancy Defect in Diamond, *Phys. Rev. Lett.* 91, 076403.



Jahn, H.A. dan Teller, E., 1937, Stability of polyatomic molecules in degenerate electronic states - I—Orbital degeneracy, *Proc. R. Soc. A 161*, 220.

Kirkley M. , 1998, *The Nature of Diamond*, Cambridge University Press, Cambridge.

Kohn, W. dan Sham, L., 1965, Self-Consistent Equations Including Exchange and Correlation Effects, *Phys. Rev. 140*, A1133-A1138.

Komarovskikh, A., Dmitriev, A., Nadolinny, V. dan Palynov, Y., 2017, A DFT calculation of EPR parameters of a germanium-vacancy defect in diamond, *Diamond & Related Materials 76* 86-89.

Krane K., 1983, *Modern Physics*. Wiley, New York.

Makov, G. dan Payne, M., 1995, Periodic boundary conditions in ab initio calculations, *Phys. Rev. B 51*, 4014.

Madelung, O., 1991, *Semiconductors: Group IV Elements and III-V Compounds*, Springer, New York.

NIMS, 2021, *PHASE: First-principles Electronic Structure Calculation Program*, <https://azuma.nims.go.jp/software/phase>, diakses 23 Maret 2021.

Prentice, J., Monserrat, B. dan Needs, R., First principles study of the dynamic Jahn-Teller distortion of the neutral vacancy in diamond, *Phys. Rev. B 95*, 014108.

Perdew, J., Burke, K., dan Ernzerhof, 1996, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett. 77*, 3865.

Perdew, J. dan Zunger, A., 1981, Self-interaction correction to density-functional approximations for many-electron systems, *Phys. Rev. B 23*, 5048.

Richardson, S. dan Harris, J., 1997, Antiquity of peridotitic diamonds from the Siberian craton, *Earth Planet. Sci. Lett. 151*, 271.

Richardson, S., Shirey S., Harris, J., dan Carlson, R., 2001, Archean subduction recorded by Re-Os isotopes in eclogitic sulfide inclusions in Kimberley diamonds, *Earth Planet. Sci. Lett. 191*.



- Rivero, P., Shelton, W., dan Meunier, V., 2006, Surface properties of hydrogenated diamond in the presence of adsorbates: A hybrid functional DFT study, *Carbon* 110 469-479.
- Sanati, M. dan Streicher, S., 2003, Defects in Silicon: the role of vibrational entrophy, *Solid State Commun.* 128, 181.
- Schirhagl, R., Chang, K., dan Loretz, M., 2014, Nitrogen-Vacancy Centers in Diamond: Nanoscale Sensors for Physics and Biology, *Annu. Rev. Phys. Chem.* 2014. 65:83–105.
- Shikata, S., Tanno, S., Teraji, T. Kanda, H., Yamada, T., dan Kushibiki, J., 2018, Precise measurements of diamond lattice constant using Bond method, *JJAP*. 57, 111301.
- Sholihun, Saito, M., Ohno, T., dan Yamasaki, T., 2015, Density-functional-theory-based calculations of formation energy and concentration of the silicon monovacancy, *Jpn. J. Appl. Phys.* 54 041301 .
- Sholihun, Kadarisman, H. P., dan Nurwantoro, P., 2018, Density-Functional-Theory Calculations of Formation Energy of the Nitrogen-Doped Diamond, *Indones. J. Chem.*, 18(4), 749-754.
- Shim, J., Lee, E., dan Niemien R., 2005, Density-functional calculations of defect formation energies using supercell methods: Defects in diamond, *Phys. Rev. B* 71, 035206.
- Straumanis, M. dan Aka, E., 1951, Precision Determination of Lattice Parameter, Coefficient of Thermal Expansion and Atomic Weight of Carbon in Diamond, *J. Am. Chem. Soc.* 1951, 73, 12, 5643–5646.
- Tolansky, S., 1962, *The history and use of diamond*, Methuen Co. Ltd, London.
- Vanpoucke, D. dan Haenen, K., 2017, Revisiting the neutral C-vacancy in diamond: Localization of electrons through DFT+U, *j.diamond*.2017.08.009.
- Wrachtrup, J. dan Jelezko, F., 2006, Processing quantum information in diamond, *J. Phys.: Condens. Matter* 18 S807.
- Wort, C. dan Balmer, R., 2008, Diamond as an electronic material, *Mat. Tod.* 11(1), 22-24.



Efek Vibrasi Fonon Terhadap Konsentrasi Vacancy Pada Intan: Kajian Komputasi Menggunakan Density Functional Theory

ZOHAN SYAH FATOMI, Sholihun, S.Si, M.Si, Ph.D.Sc;Dr.Sc. Ari Dwi Nugraheni, S.Si., M.Si.

UNIVERSITAS
GADJAH MADA

Universitas Gadjah Mada, 2021 | Diunduh dari <http://etd.repository.ugm.ac.id/>

Zelferino, A., Salustro, S., Baimo, J., Lacivita, V., Orlando, R., dan Dovesi, R., 2016,
The electronic states of the neutral vacancy in diamond: a quantum mechanical
approach, *Theor Chem Acc* 135, 74.