

## Anisotropy and Strain Energy in Decahedral Particles

A.M. Smirnov<sup>1</sup> , R.E. Shevchuk<sup>1,2</sup> , S.A. Krasnitckii<sup>1</sup> , A.E. Romanov<sup>1,3</sup> 

<sup>1</sup> ITMO University, Kronverkskiy pr., 49, bldg. A, St. Petersburg, 197101, Russia

<sup>2</sup> Baltic State Technical University «VOENMEH» named after D.F. Ustinov, 1st Krasnoarmeyskaya st. 1, St. Petersburg, 190005, Russia

<sup>3</sup> Ioffe Institute, Polytekhnicheskaya st. 26, St. Petersburg, 194021, Russia

Received: March 25, 2026

Corresponding author: [A.M. Smirnov](mailto:A.M. Smirnov)

**Abstract.** This study analyzes the strain energy stored in decahedral particles through finite-element (FE) simulations that fully account for material anisotropy. The particle is modeled as an assembly of five perfect tetrahedra with a geometrically necessary gap. A two-stage FE procedure is employed: first, prescribed displacements close the gap to generate the eigenstrain; second, the resulting stress-strain state is calculated as the elastic response arising from the introduced eigenstrain. To quantify the influence of anisotropy on the particle strain energy, we introduce an anisotropy coefficient, defined in terms of the engineering elastic constants. The numerical results are compared with isotropic analytical models based on Voigt, Reuss, and Hill homogenization schemes for a range of face-centered cubic metals. We demonstrate that isotropic approximations consistently overestimate the strain energy, the Reuss scheme provides the closest agreement to the FE solution (deviations below 26% even for highly anisotropic Pb). For weakly anisotropic materials such as Al, the considered schemes yield similar inaccuracy of approximately 8%. Our findings underscore the necessity of incorporating material anisotropy for accurate quantitative predictions of strain energy in decahedral particles.

**Acknowledgements.** This work was supported by the Russian Science Foundation (grant No. 23-72-10014).

**Citation:** Rev. Adv. Mater. Technol., 2026, vol. 8, no. 2, pp. 81–86

**View online:** <https://doi.org/10.17586/2687-0568-2026-8-2-81-86>

**View Table of Contents:** <https://reviewsamt.com/issues>

## REFERENCES

1. S. Zhou, M. Zhao, T.-H. Yang, Y. Xia. Decahedral nanocrystals of noble metals: synthesis, characterization, and applications. *Mater. Today*, 2019, vol. 22, pp. 108–131.
2. L.A. Sokura, A.M. Smirnov, A.E. Romanov. Chemical synthesis methods for controlling morphology and achieving uniform arrays of metal nanoparticles in semiconductor films. *Rev. Adv. Mater. Technol.*, 2025, vol. 7, no. 1, pp. 53–62.
3. I. Pastoriza-Santos, A. Sánchez-Iglesias, F.J. García de Abajo, L.M. Liz-Marzán. Environmental optical sensitivity of gold nanodecahedra. *Adv. Funct. Mater.*, 2007, vol. 17, no. 9, pp. 1443–1450.
4. J. Rodríguez-Fernández, C. Novo, V. Myroshnychenko, A.M. Funston, A. Sánchez-Iglesias, I. Pastoriza-Santos, J. Pérez-Juste, F.J. García de Abajo, L.M. Liz-Marzán, P. Mulvaney. Spectroscopy, imaging, and modeling of individual gold decahedra. *J. Phys. Chem. C*, 2009, vol. 113, no. 43, pp. 18623–18631.
5. S. Choi, J.A. Herron, J. Scaranto, H. Huang, Y. Wang, X. Xia, T. Lv, J. Park, H. Peng, M. Mavrikakis, Y. Xia. A comprehensive study of formic acid oxidation on palladium nanocrystals with different types of facets and twin defects. *ChemCatChem*, 2015, vol. 7, no. 14, pp. 2077–2084.
6. X. Wang, M. Vara, M. Luo, H. Huang, A. Ruditskiy, J. Park, S. Bao, J. Liu, J. Howe, M. Chi, Z. Xie, Y. Xia. Pd@Pt core-shell concave decahedra: a class of catalysts for the oxygen reduction reaction with enhanced activity and durability. *J. Am. Chem. Soc.*, 2015, vol. 137, no. 47, pp. 15036–15042.
7. H. Huang, H. Jia, Z. Liu, P. Gao, J. Zhao, Z. Luo, J. Yang, J. Zeng. Understanding of strain effects in the electrochemical reduction of CO<sub>2</sub>: using Pd nanostructures as an ideal platform. *Angew. Chemie*, 2017, vol. 129, no. 13, pp. 3648–3652.
8. W. Zhu, A. Yin, Y. Zhang, C. Yan. Highly shape-selective synthesis of monodispersed fivefold twinned platinum nanodecahedrons and nanoicosahedrons. *Chem. Eur. J.*, 2012, vol. 18, no. 39, pp. 12222–12226.
9. C.Y. Yang. Crystallography of decahedral and icosahedral particles. *J. Cryst. Growth*, 1979, vol. 47, no. 2, pp. 274–282.
10. I.A. Polonsky, A.E. Romanov, V.G. Gryaznov, A.M. Kaprelov. Disclination in an elastic sphere. *Philos. Mag. A*, 1991, vol. 64, no. 2, pp. 281–287.
11. A.E. Romanov, A.L. Kolesnikova. Elasticity boundary-value problems for straight wedge disclinations. A review on methods and results. *Rev. Adv. Mater. Technol.*, 2021, vol. 3, no. 1, pp. 55–95.
12. R.E. Shevchuk, S.A. Krasnitckii, A.E. Romanov, A.M. Smirnov. Elasticity of pentagonal wires: single disclination model versus distributed disclination model. *Lett. Mater.*, 2024, vol. 14, no. 3, pp. 175–182.
13. R.E. Shevchuk, S.A. Krasnitckii, A.M. Smirnov, A.E. Romanov. On the role of elastic anisotropy in the strain energy of decahedral metal particles: finite element analysis. *Contin. Mech. Thermodyn.*, 2026. [Submitted].
14. A.P. Sutton. *Physics of Elasticity and Crystal Defects*. Oxford University Press, Oxford, 2024.
15. W. Voigt. Ueber die beziehung zwischen den beiden elasticitätsconstanten isotroper körper. *Ann. Phys.*, 1889, vol. 274, no. 12, pp. 573–587. [In German].
16. A. Reuss. Berechnung der fließgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle. *Z. Angew. Math. Mech.*, 1929, vol. 9, no. 1, pp. 49–58. [In German].
17. R. Hill. The elastic behaviour of a crystalline aggregate. *Proc. Phys. Soc. A*, 1952, vol. 65, no. 5, pp. 349–354.
18. G. Simmons, H. Wang. *Single Crystal Elastic Constants and Calculated Aggregate Properties. A Handbook. Second Edition*. The MIT Press, Cambridge, Massachusetts, London, 1971.
19. B.-J. Lee, J.-H. Shim, M.I. Baskes. Semiempirical atomic potentials for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, Al, and Pb based on first and second nearest-neighbor modified embedded atom method. *Phys. Rev. B*, 2003, vol. 68, no. 14, art. no. 144112.
20. S. Patala, L.D. Marks, M. Olvera de la Cruz. Elastic strain energy effects in faceted decahedral nanoparticles. *J. Phys. Chem. C*, 2013, vol. 117, no. 3, pp. 1485–1494.