Paul-Drude-Institut für Festkörperelektronik

Master Thesis Topic

Diamond in a Drop: Modeling Low-Pressure Growth in Liquid Metals

Why Diamond Matters

Diamond Isn't Just for Jewelry — It's the Future of Quantum Tech!

From quantum sensors to qubits, diamond's unmatched properties — extreme hardness, biocompatibility radiation resistance, and record-breaking thermal conductivity — make it a superstar material for next-gen technologies. But growing diamond sustainably, and at low pressure, is a game-changer. This thesis explores how carbon atoms turn into diamonds in liquid metal systems, using atomistic simulations to uncover the atomic magic behind a process that could reshape the future of quantum materials.

Your Mission

- Study how carbon behaves in molten metal alloys (Ga–Fe–Ni–Si) at moderate temperatures and atmospheric pressure.
- Explore key factors (supersaturation, bonding, surface effects) that control the formation of diamond (sp^3) vs. graphite (sp^2).
- Provide theoretical insights to guide experimental efforts in low-pressure diamond synthesis with liquid metal catalysts.

Expected Outcomes

- A validated atomistic simulation workflow for modeling carbon transport and nucleation in molten metal systems.
- Practical recommendations (a "growth recipe") for enhancing low-pressure, seed-free diamond growth with liquid metal catalysts.
- Potential contribution to a peer-reviewed publication and poster presentation on key findings.

Skills You'll build

- **DFT Calculations:** Learn to perform density functional theory calculations to analyze material behaviors.
- **Molecular Dynamics Simulations:** Gain hands-on experience running simulations to study atomic and molecular dynamics.
- **Experience with Supercomputers:** Utilize high-performance computing (HPC) systems to run large-scale simulations
- **Scientific Communication:** Develop the ability to present and publish your research findings in a professional context.
- **Collaborative Research:** Work in a collaborative environment that fosters teamwork and idea-sharing.

Your Profile

- Bachelor's degree in materials science, physics, or a related field
- (Optional) Background in Programming skill using such as Python and familiarity with Linux/Unix environments

- Effective communication skills in english and a genuine enthusiasm for contributing to cutting-edge research in the field of materials science.

Opportunities and Benefits

- Unique theory/simulation capabilities
- Modern laboratories with a wide range of experimental techniques
- Supportive environment with experts for various scientific sub-fields
- International and culturally diverse community
- Location in the heart of Berlin with excellent public transport connections, a subsidized travel ticket
- Possibility to participate in professional development programs

Contact

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