

Solve the Hard Problem: Materials Harder than Diamond

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Hypotheses of interest

Hypothesis 1: Materials that are harder than diamond are possible to achieve.

 Hypothesis 2: If one or more harder than diamond materials existed, there would be high impact energy applications for them.



What is hardness?

Metrics associated with hardness - Wear resistance Diamond Graphite – Ductility - Strength - Stiffness How is it measured? Indentation size & depth - Scratch - Rebound

Photo credit: taken from "Eight Allotropes of Carbon" Michael Ströck - Created by Michael Ströck. Licensed under CC BY-SA 3.0 via Wikimedia Commons



Harder than diamond



Figure adapted from: Kanyanta, Valentine. "Hard, Superhard and Ultrahard Materials: An Overview." Microstructure-Property Correlations for Hard, Superhard, and Ultrahard Materials. Springer International Publishing, 2016. 1-23.



Emerging "harder than diamond" materials show promise?

| Material | Vickers Hardness (GPa) | Stage of Verification |
|----------------------|---------------------------------------|--|
| Fullerite | 200 - 300 ¹ | Experimental |
| Nano-twinned diamond | 200 ² | Experimental |
| Q-Carbon | 60% harder than diamond ³ | Extrapolated from theory and nano-indentation experimentation on filament samples |
| Lonsdaleite | 152 ⁴ | Theoretical |
| Diamond | 115 ⁴ | |
| Nano-twinned c-BN | About as hard as diamond ⁵ | Experimental |
| w-BN | About as hard as diamond ⁶ | Experimental |

Harder than diamond?

- ➢ Fullerite
- Nano-twinned diamond
- Q-Carbon
- Lonsdaleite
- Nano-twinned c-BN

≻ w-BN

1: Popov, M., et al. "Synthesis of ultrahard fullerite with a catalytic 3D polymerization reaction of C 60." Carbon 76 (2014): 250-256.

2: Huang, Quan, et al. "Nanotwinned diamond with unprecedented hardness and stability." Nature 510.7504 (2014): 250-253.

3: Narayan, Jagdish, and Anagh Bhaumik. "Novel phase of carbon, ferromagnetism, and conversion into diamond." Journal of Applied Physics 118.21 (2015): 215303. 4: Kanyanta, Valentine. "Microstructure-Property Correlations for Hard, Superhard, and Ultrahard Materials." (2016).

5: Tian, Yongjun, et al. "Ultrahard nanotwinned cubic boron nitride." Nature 493.7432 (2013): 385-388.

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6: Pan, Zicheng, et al. "Harder than diamond: superior indentation strength of wurtzite BN and lonsdaleite." Physical review letters 102.5 (2009): 055503

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If HTD materials were successfully developed, what energy applications would they impact?

Hypotheses:

- Drilling (Geothermal, O&G)
- Mining comminution and grinding
- Cutting tools for vehicle lightweighting materials
- Vehicle powertrain low friction, wear resistant coatings

– Others?



Better (hotter) geothermal resources tend to be deeper. The combination of deeper and hotter is challenging for drill bits



Temperatures of geothermal resources at various depths in the continental U.S¹







Worn bit after removal at ~2000 ft ³

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 Renner, J. L. The Future of Geothermal Energy. No. INL/EXT-06-11746. Idaho National Laboratory (INL), 2006.
Kipsang, Carolyn. "Cost model for geothermal wells." (2014).
Bit image from: Raymond, David, et al. "PDC Bits Outperform Conventional Bit in Geothermal Drilling Project." Geothermal Resources Council Transactions 36 (2012): 307-316.

Mining comminution is energy intensive and inefficient



U.S. mining industry energy consumption by process in 2006

Grinding and crushing operations consume a

These operations are very inefficient with

1: DOE, US. "Mining industry energy bandwidth study." US Department of Energy, Washington, DC (2007).

2: Tromans, Desmond. "Mineral comminution: energy efficiency considerations." Minerals engineering 21.8 (2008): 613-620.

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Can HTD materials lead to more efficient comminution?

Energy use increases exponentially as smaller final particle sizes are required¹

1000 Ultrafine Specific energy input, kWh/t 00 Fine Intermediate Coarse 0.1 0.1 10 100 1000 10000 Product size, µm

Can harder than diamond materials improve the efficiency of crushing and/or grinding?



Required energy for size reduction in comminution

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1: Wang, Yanmin, and Eric Forssberg. "Enhancement of energy efficiency for mechanical production of fine and ultra-fine particles in comminution." China Particuology 5.3 (2007): 193-201.

2: Crushing image credit: "Infographic - Counting the Cost of Comminution." Mining Technology. N.p., n.d. Web. 23 Feb. 2017. 3: Grinding image credit: Khadka, Prakash, et al. "Pharmaceutical particle technologies: an approach to improve drug solubility, dissolution and bioavailability." asian journal of pharmaceutical sciences 9.6 (2014): 304-316.

Automotive & aerospace industries aim for lightweighting, which would have large energy impact

Significant increase in titanium usage in aircraft...



Figure adapted from: Bowden, David M., and William H. Peter. Near-net shape fabrication using low-cost titanium alloy powders. The Boeing Company, 2012.

...& aluminum in automotive vehicles (e.g. Ford F150)



Siler, Steve. "2015 Ford F-150 Brings Aluminum and LEDs to the 2014 Detroit Auto Show." NY Daily News. N.p., 13 Jan. 2014.

- Advanced tool insert materials (PCD) have a limited tool life
- High stresses and elevated temperatures at the cutting region
- 80% of the heat of cutting Ti is transferred to the tool ²
- Reduce machining time and lubricant requirements
- Cutting costs may be reduced by 15-30%^{3,4}



* Based on analysis in ARPA-E METALS FOA. Replacement constrained by achieving equivalent bending stress. Only use phase is considered in fuel savings, not energy embedded in metals themselves. February 28, 2017

Call to action!

- We want your input!
 - Emerging materials "harder than diamond"
 - Fundamental limitation to reaching low cost
 - Identified energy impact applications
 - Other energy applications utilizing HTD materials

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