Harder than Diamond?

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Beautiful
Expensive
Hardest crystal
However, even diamond has limitations.
It cannot cut ferrous metals[1], because of a chemical reaction that produces iron carbide. A ferrous metal is a metal that contains iron, such as steel.
Besides, another question: If we can find a material which is harder than diamond, is that great?
We are looking for a material, which is harder than diamond and can cut ferrous metals.
Which system should we focus first?

**Carbon Nitrides**

Why?
**Carbon Nitrides** were long believed to have materials harder than diamond [2].

- **C-C bond length**: 1.55 Å
- **C-N bond length**: 1.47 Å
The next step

To find out the hardest structure of the C-N system.
How to find out the hardest structure?

1. Find out all the stable structures
2. Calculate their hardness
3. Find out the hardest structure

USPEX

Based on *ab initio* evolutionary algorithm

It can deal with complex systems (using supercomputer)

Micro Model

Macro Model

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What we found?
Hardness compare with diamond and steel

Super-hard
Harder than Diamond?

In conclusion, we find Carbon nitrides is harder than BN, which is the second hardest crystal in the world, and are much harder than steel. They can be used in industry.
Dear friends, thank you!

Reference