

Diamond

The world's favourite gem

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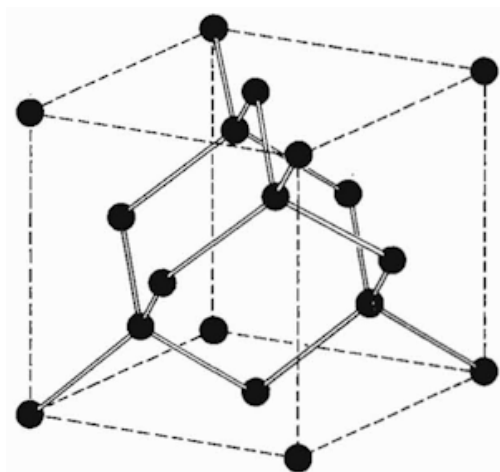
Molecule of the Month July 1996

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Also available: [JSMol](#) version.

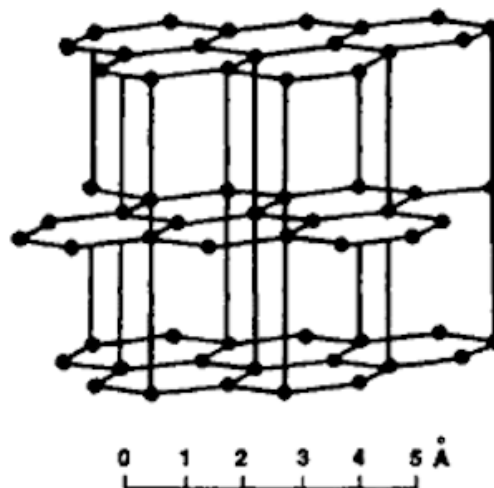
Its properties

Diamond has been [prized for centuries](#) as a gemstone of exceptional brilliance and lustre. But to a scientist, diamond is interesting for its range of exceptional and extreme properties. When compared to almost any other material, diamond almost always comes out on top. As well as being the hardest known material, it is also the least compressible, and the stiffest material, the best thermal conductor with an extremely low thermal expansion, chemically inert to most acids and alkalis, transparent from the deep uv through the visible to the far infrared, and is one of the few materials known with a *negative* electron affinity (or work function).



Diamond lattice.

The C atoms are 4-coordinate and arranged tetrahedrally in a strong 3D structure.



Graphite lattice.

The C atoms are 3 coordinate and arranged hexagonally in 2D layers.

There are strong bonds within the layers but weak ones between layers allowing the layers to slip past each other easily.

Choose virtually any characteristic of a material - electronic, structural, or optical - and the value associated with diamond will almost always be the most extreme: Diamond is invariably '*the biggest and the best*'. The following is a table of the properties of diamond that render it so potentially useful across many fields of science.

Property	Value	Units
Hardness	10,000	kg/mm ²
Strength, tensile	>1.2	GPa
Strength, compressive	>110	GPa
Sound velocity	18,000	m/s
Density	3.52	g/cm ³
Young's modulus	1220	GPa
Poisson's ratio	0.2	Dimensionless

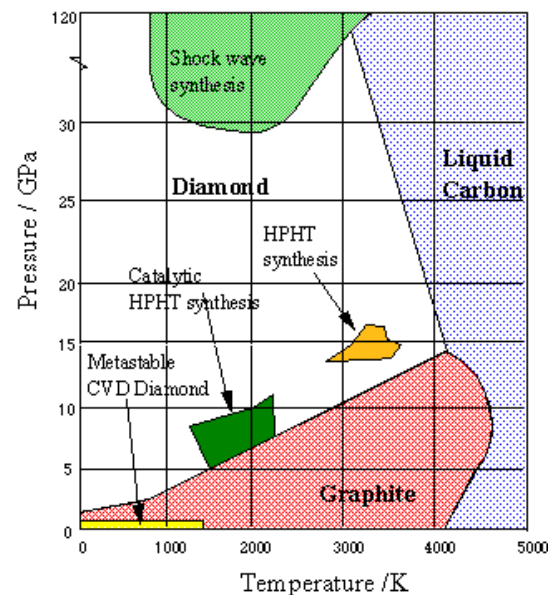
Thermal expansion coefficient	0.0000011	/K
Thermal conductivity	20.0	W/cm-K
Thermal shock parameter	30,000,000	W/m
Debye temperature	2,200	K
Optical index of refraction (at 591 nm)	2.41	Dimensionless
Optical transmissivity (from nm to far IR)	225	Dimensionless
Loss tangent at 40 Hz	0.0006	Dimensionless
Dielectric constant	5.7	Dimensionless
Dielectric strength	10,000,000	V/cm
Electron mobility	2,200	cm ² /V-s
Hole mobility	1,600	cm ² /V-s
Electron saturated velocity	27,000,000	cm/s
Hole saturated velocity	10,000,000	cm/s
Work function	small and negative	(On [111] surface)
Bandgap	5.45	eV
Resistivity	10 ¹³ - 10 ¹⁶	Ohm-cm

Diamond and Graphite

Diamond is composed of the single element carbon, and it is the arrangement of the C atoms in the lattice that give diamond its amazing properties. Compare the structure of diamond and graphite, both composed of just carbon. In diamond we have the hardest known material, in graphite we have one of the softest, simply by rearranging the way the atoms are bonded together.

The relationship between diamond and graphite is a thermodynamic and kinetic one, as can be seen in the phase diagram for carbon (right). At normal temperatures and pressures, graphite is only a few eV more stable than diamond, and the fact that diamond exists at all is due to the very large activation barrier for conversion between the two. There is no easy mechanism to convert between the two and so interconversion requires almost as much energy as destroying the entire lattice and rebuilding it. Once diamond is formed, therefore, it cannot reconvert back to graphite because the barrier is too high. So diamond is said to be *metastable*, since it is *kinetically stable*, not *thermodynamically stable*.

Diamond is created deep underground under conditions of extreme pressure and temperature. Under these conditions diamond is actually the more stable of the two forms of carbon, and so over a period of millions of years carbonaceous deposits slowly crystallise into single crystal diamond gemstones.



Natural diamonds

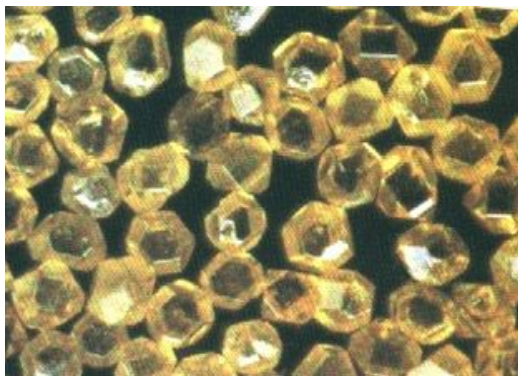
Natural diamonds are classified by the type and level of impurities found within them.

- **Type Ia diamond** - Most natural diamonds are of this type, which contain up to 0.3% nitrogen.
- **Type Ib diamond** - Very rare (~0.1%) in nature, but almost all synthetic (industrial) diamonds are of this type. They contain nitrogen at concentrations of up to 500 ppm.
- **Type IIa diamond** - Very rare in nature, these diamonds contain so little nitrogen that it can't be easily detected by the usual IR or UV absorption measurements.
- **Type IIb diamond** - Extremely rare in nature. These have such a low concentration of nitrogen (even lower than type IIa) that the crystal is a p-type



Diamond gemstones can come in variety of colours depending on impurities such as B, N, and vacancy defects within the diamond lattice, along with a variety of different cuts to reflect light and make them sparkle.

semiconductor (due to uncompensated B acceptor impurities).



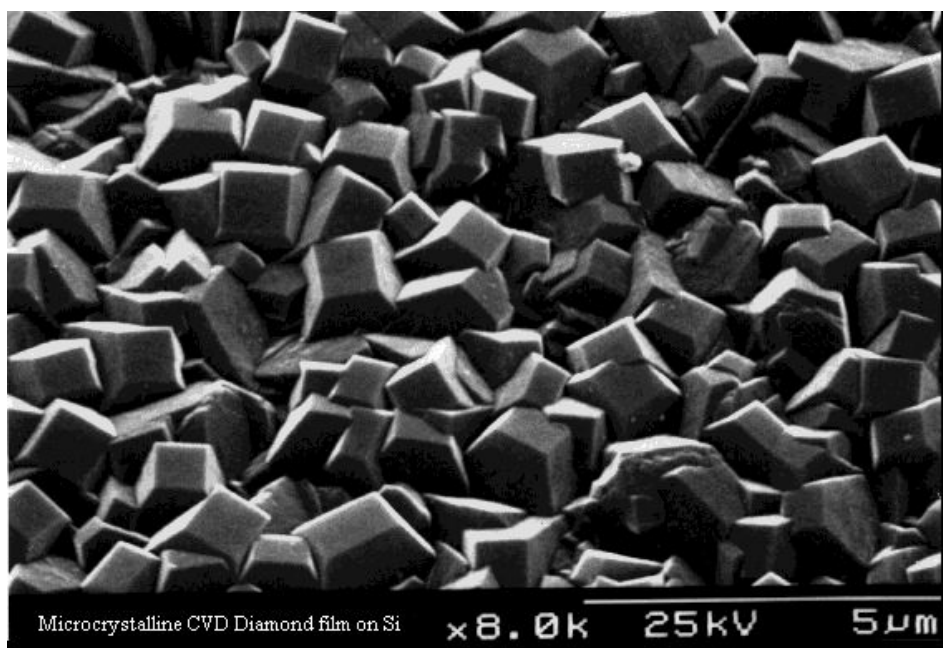
HPHT 'industrial' diamonds.
They are slightly yellow due to N impurities,
which makes them useless for jewellery
but is no problem for abrasive applications.

Synthetic Industrial Diamond

These have been made since the early 1950's, by a process called **High Pressure High Temperature synthesis** (HPHT). This is an attempt to mimic the conditions under which natural diamond forms deep in the earth. Graphite is put into a huge hydraulic press at high temperatures and pressures, and with the addition of a metallic catalyst, converts to diamond over a period of a few hours. The diamond crystals that are produced by this method are typically a few mm in size, which are too flawed for use as gemstones, but are extremely useful as hard-wearing edges on cutting tools and drill-bits.

Thin Film Diamond

This is a relatively recent development (since ~1990), which allows thin films (nm to mm) of polycrystalline diamond to be deposited onto a range of materials, using a technique called **Chemical Vapour Deposition** (CVD). This is creating a great deal of excitement in the academic community, since for the first time we have access to all the superlative properties of diamond in a form that is useful for engineering applications. We can imagine hard-wearing diamond coatings on machine parts, diamond windows, diamond electronics, diamond displays, diamond fibre reinforcements, and a whole host of other applications. A review of the recent developments in this area can be found [here](#).



A CVD polycrystalline diamond film from the [Bristol CVD diamond lab](#).

References

1. J.E. Field, *The Properties of Natural and Synthetic Diamond*, Academic Press, London, 1992.
2. F.P. Bundy, *The P,T Phase and Reaction diagram for elemental Carbon*, 1979; *J. Geophys. Res.* **85 (B12)** (1980) 6930.
3. Spear and Dismukes *Synthetic Diamond - Emerging CVD Science and Technology*: Wiley, NY, 1994.