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DATE 20 January 2008

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FROM Charles R. Anderson, Ph.D.

SUBJ XPS Analysis of the Surface of a White Sona Diamond Simulant, Round Cut, 0.5 Carat, 5 mm Size to Determine its Composition

Summary

The principal results on the Sona diamond simulant, after being cleaned with Windex, acetone, rubbed on acetone-soaked paper, rinsed with acetone, rinsed with isopropyl alcohol, and sputtered with Ar ions to remove the outer 20 nm of material were:

1. The gemstone is yttrium-stabilized cubic zirconia primarily. It appears to have either a very small concentration of Mo or a larger concentration of S in it near the surface, with Mo appearing to be more likely. The ambiguity is due to the small amounts and some unfortunate peak overlaps.

2. No aluminum was found, therefore there is no sapphire infused into this surface. The carbon concentration was very low after the sputter removal of only 20 nm, so no significant diamond material could be infused into the gemstone surface.

3. This gemstone was oxygen-enriched, not slightly deficient the way many other cubic zirconia gemstones are. This probably means that some carbon dioxide and water have reacted with the Zr in the near surface region, which commonly does occur with zirconia in time.

Samples

A loose white round-cut, 0.5 carat weight, 5 mm Sona diamond simulant gemstone from C3jewelry, Atlanta, GA, www.sonadiamond.com was ordered by Charles Anderson on 7 Dec 07. It was received on 10 Dec 07 at Anderson Materials Evaluation, Inc. with a card giving its color as D-E and its clarity as VVS-1. It was wrapped in blue paper with an outer wrap of white, thick paper noting that it was made in Israel. It was cleaned with Windex, the blue version with Ammonia-D. Then it was rinsed with acetone, rubbed several times over an acetone-soaked paper surface, rinsed with acetone, and finally rinsed with isopropyl alcohol. Once in the analysis chamber of the XPS system, it was argon ion sputtered with 4 KeV ions using a differentially pumped and rastered ion gun for sufficient time that 20 nm of material would have been removed from SiO_2. Other materials will sputter at somewhat different rates, with organic surface contaminants generally sputtering faster than SiO_2. Then the broad front surface was analyzed with XPS to determine it elemental composition.

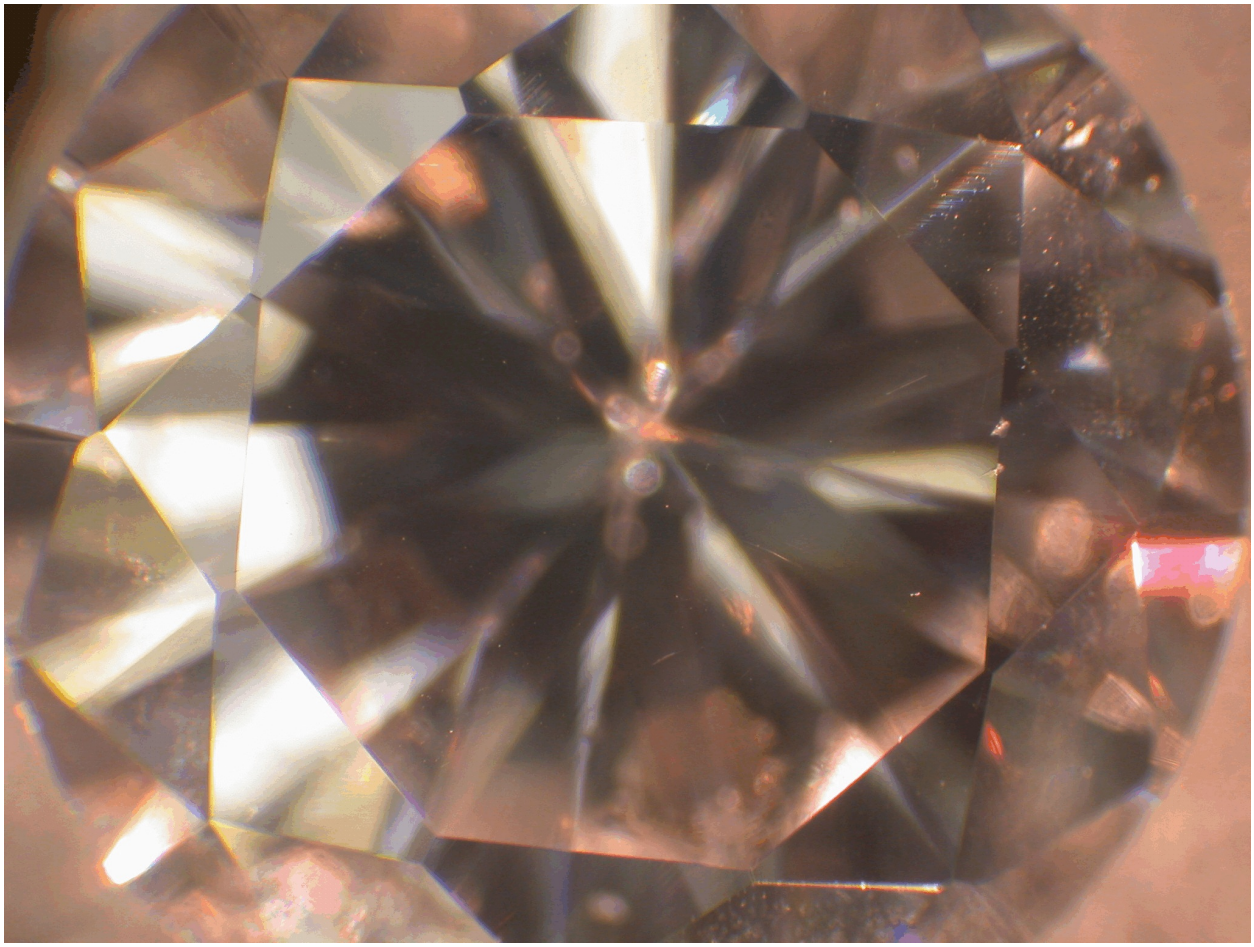

Fig. 1. The round cut Sona diamond simulant gemstone analyzed with XPS as mounted for XPS analysis. The analysis area was on the top surface as shown. The front surface was rubbed with acetone-soaked paper, which helped to clean off organic contaminants.

XPS Results

The surface of the front face of the Sona diamond simulant after cleaning was examined with XPS using a monochromatic aluminum x-ray source. The quantitative elemental concentration results were obtained from an elemental survey spectrum covering the binding energy range from 0 to 1100 eV with a step size of 0.5 eV and a long 4-hour data acquisition time for improved accuracy and sensitivity. The quantitative elemental concentration results for the surface are reported in Table 1.

Table 1. The elemental concentrations (in atomic %) of the front face surface of the Sona diamond simulant gemstone.

Element	Sona Gemstone after Cleaning & Sputtering to Remove 20 nm
O	60.333
C	9.713
Zr	21.340
Y	6.320
Mo	0.834
Ar	1.461
Y: Zr Ratio	0.296

The Sona diamond simulant is basically a yttrium-stabilized cubic zirconia with a yttrium to zirconium ratio which is common for such gemstone materials. It appears to have the formula:

$$ZrO_2 \bullet 0.148\ Y_2O_3 \bullet 0.039\ MoO_2 \bullet 0.15\ CO_2 \bullet 0.15\ H_2O$$

It does not have the oxygen-deficient chemistry found in some cubic zirconia gemstones, but instead has a surplus of oxygen. It is possible that the photoelectron peak taken to be Mo is instead S. The ambiguity is due to an electron energy loss peak from the Y 3d photoelectron peak obscuring the S 2p and a host of photoelectron peak and loss peak overlaps for various Zr and Y peaks with the smaller Mo peaks. Because Mo has a XO_2 favored oxide just as Zr does, it seems reasonable that this peak is Mo, but sulfur should not be entirely ruled out. MoO_2 has a somewhat lead gray color. To my admittedly untrained eye, this gemstone does appear to have a very slight gray tint. Molybdenum also has a Mo_2O_3 oxide, but this seems usually to be more rare. If the Mo takes that form, then it substitutes for the Y, rather than the Zr atoms in the gemstone structure. The Mo_2O_3

oxide would use a bit less of the oxygen and its coloration is black, probably making it less desirable.

There is no evidence for aluminum in the spectrum and it would have been readily observed if it were present. Because of this, there is no sapphire, which is aluminum oxide, infused into the near surface region of this gemstone. Because 20 nm of material was sputtered, it might be possible that the outer 20 nm of material had some Al, but for the fact that I took a spectrum before sputtering and saw none then either. The sputtering did remove significant carbon, but it is most likely that that was just due to the usual adventitious carbon absorbed from the air.