# On the Origin of Chemically Graded Metal/Ceramic Interface

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Table S1: The space group, lattice parameters, and Wyckoff positions of metal and carbon atoms in carbides.

| Structure | Lattice Parameters | | | | | | Wyckoff positions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | a (Å) | b (Å) | c (Å) | $\alpha$ | $\beta$ | $\gamma$ | Atom | Site | x | y | z |
| TiC ($Fm\bar{3}m$) | 4.335 | 4.335 | 4.335 | 90 | 90 | 90 | Ti | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | C | 4b | 0.500 | 0.500 | 0.500 |
| ZrC ($Fm\bar{3}m$) | 4.711 | 4.711 | 4.711 | 90 | 90 | 90 | Zr | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | C | 4b | 0.500 | 0.500 | 0.500 |
| HfC ($Fm\bar{3}m$) | 4.647 | 4.647 | 4.647 | 90 | 90 | 90 | Hf | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | C | 4b | 0.500 | 0.500 | 0.500 |
| $V_6C_5$ ($P3_11\bar{2}$) | 10.211 | 10.211 | 14.358 | 90 | 90 | 120 | V | 6c | 0.111 | 0.528 | 0.749 |
| Trigonal 151 | | | | | | | V | 6c | 0.111 | 0.247 | 0.924 |
| | | | | | | | V | 6c | 0.471 | 0.221 | 0.252 |
| | | | | | | | C | 3a | 0.108 | 0.215 | 0.667 |
| | | | | | | | C | 3b | 0.109 | 0.555 | 0.500 |
| | | | | | | | C | 3a | 0.111 | 0.556 | 0.000 |
| | | | | | | | C | 3a | 0.439 | 0.219 | 0.000 |
| | | | | | | | C | 3b | 0.442 | 0.221 | 0.500 |
| $Nb_6C_5$ (C2/m) | 5.525 | 9.547 | 5.507 | 90 | 109.648 | 90 | Nb | 8j | 0.240 | 0.323 | 0.746 |
| Monoclinic 12 | | | | | | | Nb | 4i | 0.236 | 0.500 | 0.264 |
| | | | | | | | C | 4h | 0.000 | 0.167 | 0.500 |
| | | | | | | | C | 4g | 0.000 | 0.335 | 0.000 |
| | | | | | | | C | 2d | 0.000 | 0.500 | 0.500 |
| $Ta_2C$ ($P\bar{3}m1$) | 3.123 | 3.123 | 4.963 | 90 | 90 | 120 | Ta | 2d | 0.333 | 0.667 | 0.252 |
| Trigonal 164 | | | | | | | C | 1a | 0.000 | 0.000 | 0.000 |
| $Mg_2C_3$ (Pnnm) | 5.294 | 6.449 | 3.740 | 90 | 90 | 90 | Mg | 4g | 0.108 | 0.791 | 0.500 |
| Orthorhombic 58 | | | | | | | C | 4g | 0.207 | 0.618 | 0.000 |
| | | | | | | | C | 2c | 0.000 | 0.500 | 0.000 |
| $Al_4C_3$ ($R\bar{3}m$) | 3.354 | 3.354 | 25.117 | 90 | 90 | 120 | Al | 6c | 0.000 | 0.000 | 0.130 |
| Trigonal 166 | | | | | | | Al | 6c | 0.000 | 0.000 | 0.293 |
| | | | | | | | C | 6c | 0.000 | 0.000 | 0.217 |
| | | | | | | | C | 3a | 0.000 | 0.000 | 0.000 |
| $Cr_3C_2$ (Pnma) | 5.474 | 2.789 | 11.466 | 90 | 90 | 90 | Cr | 4c | 0.017 | 0.750 | 0.403 |
| Orthorhombic 62 | | | | | | | Cr | 4c | 0.134 | 0.250 | 0.068 |
| | | | | | | | Cr | 4c | 0.184 | 0.750 | 0.774 |
| | | | | | | | C | 4c | 0.101 | 0.750 | 0.202 |
| | | | | | | | C | 4c | 0.237 | 0.750 | 0.951 |
| $Fe_3C$ (Pnma) | 5.026 | 6.720 | 4.480 | 90 | 90 | 90 | Fe | 8d | 0.177 | 0.068 | 0.332 |
| Orthorhombic 62 | | | | | | | Fe | 4c | 0.037 | 0.250 | 0.837 |
| | | | | | | | C | 4c | 0.123 | 0.750 | 0.561 |

Table S2: The space group, lattice parameters, and Wyckoff positions of metal and nitrogen atoms in nitrides.

| Structure | Lattice Parameters | | | | | | Wyckoff positions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | a (Å) | b (Å) | c (Å) | $\alpha$ | $\beta$ | $\gamma$ | Atom | Site | x | y | z |
| TiN ($Fm\bar{3}m$) | 4.252 | 4.252 | 4.252 | 90 | 90 | 90 | Ti | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | N | 4b | 0.500 | 0.500 | 0.500 |
| ZrN ($Fm\bar{3}m$) | 4.595 | 4.595 | 4.595 | 90 | 90 | 90 | Zr | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | N | 4b | 0.500 | 0.500 | 0.500 |
| HfN ($Fm\bar{3}m$) | 4.533 | 4.533 | 4.533 | 90 | 90 | 90 | Hf | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | N | 4b | 0.500 | 0.500 | 0.500 |
| VN ($P6_3/mmc$) | 2.776 | 2.776 | 5.164 | 90 | 90 | 120 | V | 2d | 0.333 | 0.667 | 0.750 |
| Hexagonal 194 | | | | | | | N | 2a | 0.000 | 0.000 | 0.500 |
| NbN ($P\bar{6}m2$) | 2.976 | 2.976 | 2.901 | 90 | 90 | 120 | Nb | 1a | 0.000 | 0.000 | 0.000 |
| Hexagonal 187 | | | | | | | N | 1d | 0.333 | 0.667 | 0.500 |
| TaN ($P\bar{6}2m$) | 5.235 | 5.235 | 2.920 | 90 | 90 | 120 | Ta | 1a | 0.000 | 0.000 | 0.000 |
| Hexagonal 189 | | | | | | | Ta | 2d | 0.333 | 0.667 | 0.500 |
| | | | | | | | N | 3f | 0.392 | 0.000 | 0.000 |
| $Mg_3N_2$ (Ia-3) | 10.023 | 10.023 | 10.023 | 90 | 90 | 90 | Mg | 48e | 0.118 | 0.889 | 0.153 |
| Cubic 206 | | | | | | | N | 8b | 0.750 | 0.250 | 0.750 |
| | | | | | | | N | 24d | 0.969 | 0.500 | 0.750 |
| AlN ($P6_3mc$) | 3.129 | 3.129 | 5.017 | 90 | 90 | 120 | Al | 2b | 0.667 | 0.333 | 0.499 |
| Hexagonal 186 | | | | | | | N | 2b | 0.667 | 0.333 | 0.881 |
| CrN ($F\bar{4}3m$) | 4.388 | 4.388 | 4.388 | 90 | 90 | 90 | Cr | 4c | 0.250 | 0.250 | 0.250 |
| Cubic 216 | | | | | | | N | 4a | 0.000 | 0.000 | 0.000 |
| FeN ($F\bar{4}3m$) | 4.224 | 4.224 | 4.224 | 90 | 90 | 90 | Fe | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 216 | | | | | | | N | 4d | 0.750 | 0.750 | 0.750 |

Table S3: The space group, lattice parameters, and Wyckoff positions of metal and oxygen atoms in oxides.

| Structure | Lattice Parameters | | | | | | Wyckoff positions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | a (Å) | b (Å) | c (Å) | $\alpha$ | $\beta$ | $\gamma$ | Atom | Site | x | y | z |
| $TiO_2$ ($I4_1/amd$) | 3.803 | 3.803 | 9.739 | 90 | 90 | 90 | Ti | 4a | 0.000 | 0.000 | 0.000 |
| Tetragonal 141 | | | | | | | O | 8e | 0.500 | 0.500 | 0.706 |
| $ZrO_2$ ($P2_1/c$) | 5.194 | 5.242 | 5.382 | 90 | 99.688 | 90 | Zr | 4e | 0.724 | 0.456 | 0.290 |
| Monoclinic 14 | | | | | | | O | 4e | 0.935 | 0.325 | 0.649 |
| | | | | | | | O | 4e | 0.549 | 0.757 | 0.525 |
| $HfO_2$ ($P2_1/c$) | 5.139 | 5.192 | 5.323 | 90 | 99.679 | 90 | Hf | 4e | 0.724 | 0.457 | 0.292 |
| Monoclinic 14 | | | | | | | O | 4e | 0.932 | 0.330 | 0.653 |
| | | | | | | | O | 4e | 0.551 | 0.757 | 0.522 |
| $V_2O_3$ ($R\bar{3}c$) | 5.127 | 5.127 | 14.136 | 90 | 90 | 120 | V | 12c | 0.000 | 0.000 | 0.351 |
| Trigonal 167 | | | | | | | O | 18e | 0.303 | 0.000 | 0.250 |
| $Nb_2O_5$ (C2/m) | 13.090 | 3.872 | 4.059 | 90 | 90.737 | 90 | Nb | 4i | 0.146 | 0.000 | 0.068 |
| Monoclinic 12 | | | | | | | O | 4i | 0.852 | 0.000 | 0.489 |
| | | | | | | | O | 4i | 0.815 | 0.500 | 0.996 |
| | | | | | | | O | 2a | 0.000 | 0.000 | 0.000 |
| $Ta_2O_5$ (C2/c) | 12.942 | 4.928 | 5.595 | 90 | 103.155 | 90 | Ta | 8f | 0.141 | 0.246 | 0.769 |
| Monoclinic 15 | | | | | | | O | 8f | 0.888 | 0.550 | 0.517 |
| | | | | | | | O | 8f | 0.795 | 0.932 | 0.872 |
| | | | | | | | O | 4e | 0.000 | 0.891 | 0.250 |
| MgO ($Fm\bar{3}m$) | 4.256 | 4.256 | 4.256 | 90 | 90 | 90 | Mg | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | O | 4b | 0.500 | 0.500 | 0.500 |
| $Al_2O_3$ ($R\bar{3}c$) | 4.808 | 4.808 | 13.122 | 90 | 90 | 120 | Al | 12c | 0.000 | 0.000 | 0.352 |
| Trigonal 167 | | | | | | | O | 18e | 0.306 | 0.000 | 0.250 |
| $Cr_2O_3$ ($R\bar{3}c$) | 5.063 | 5.063 | 13.848 | 90 | 90 | 120 | Cr | 12c | 0.000 | 0.000 | 0.348 |
| Trigonal 167 | | | | | | | O | 18e | 0.304 | 0.000 | 0.250 |
| $Fe_2O_3$ ($R\bar{3}c$) | 5.097 | 5.097 | 13.910 | 90 | 90 | 120 | Fe | 12c | 0.000 | 0.000 | 0.354 |
| Trigonal 167 | | | | | | | O | 18e | 0.695 | 0.000 | 0.250 |

Table S4: The space group, lattice parameters, and Wyckoff positions of metal atoms and octahedral (oct) and tetrahedral (tet) sites.

| Structure | Lattice Parameters | | | | | | Wyckoff positions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | a (Å) | b (Å) | c (Å) | $\alpha$ | $\beta$ | $\gamma$ | Atom | Site | x | y | z |
| Ti ($P6_3/mmc$) | 2.935 | 2.935 | 4.647 | 90 | 90 | 120 | Ti | 2c | 0.333 | 0.666 | 0.250 |
| Hexagonal 194 | | | | | | | C/N/O | 2a (oct) | 0.000 | 0.000 | 0.000 |
| | | | | | | | C/N/O | 4f (tet) | 0.333 | 0.666 | 0.625 |
| Zr ($P6_3/mmc$) | 3.230 | 3.230 | 5.172 | 90 | 90 | 120 | Zr | 2c | 0.333 | 0.666 | 0.250 |
| Hexagonal 194 | | | | | | | C/N/O | 2a (oct) | 0.000 | 0.000 | 0.000 |
| | | | | | | | C/N/O | 4f (tet) | 0.333 | 0.666 | 0.625 |
| Hf ($P6_3/mmc$) | 3.199 | 3.199 | 5.054 | 90 | 90 | 120 | Hf | 2c | 0.333 | 0.666 | 0.250 |
| Hexagonal 194 | | | | | | | C/N/O | 2a (oct) | 0.000 | 0.000 | 0.000 |
| | | | | | | | C/N/O | 4f (tet) | 0.333 | 0.666 | 0.625 |
| V ($Im\bar{3}m$) | 2.999 | 2.999 | 2.999 | 90 | 90 | 90 | V | 2a | 0.000 | 0.000 | 0.000 |
| Cubic 229 | | | | | | | C/N/O | 6b (oct) | 0.000 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 12d (tet) | 0.250 | 0.000 | 0.500 |
| Nb ($Im\bar{3}m$) | 3.320 | 3.320 | 3.320 | 90 | 90 | 90 | Nb | 2a | 0.000 | 0.000 | 0.000 |
| Cubic 229 | | | | | | | C/N/O | 6b (oct) | 0.000 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 12d (tet) | 0.250 | 0.000 | 0.500 |
| Ta ($Im\bar{3}m$) | 3.319 | 3.319 | 3.319 | 90 | 90 | 90 | Ta | 2a | 0.000 | 0.000 | 0.000 |
| Cubic 229 | | | | | | | C/N/O | 6b (oct) | 0.000 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 12d (tet) | 0.250 | 0.000 | 0.500 |
| Mg ($P6_3/mmc$) | 3.189 | 3.189 | 5.193 | 90 | 90 | 120 | Mg | 2c | 0.333 | 0.666 | 0.250 |
| Hexagonal 194 | | | | | | | C/N/O | 2a (oct) | 0.000 | 0.000 | 0.000 |
| | | | | | | | C/N/O | 4f (tet) | 0.333 | 0.666 | 0.625 |
| Al ($Fm\bar{3}m$) | 4.037 | 4.037 | 4.037 | 90 | 90 | 90 | Al | 4a | 0.000 | 0.000 | 0.000 |
| Cubic 225 | | | | | | | C/N/O | 4b (oct) | 0.500 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 8c (tet) | 0.250 | 0.250 | 0.250 |
| Cr ($Im\bar{3}m$) | 2.842 | 2.842 | 2.842 | 90 | 90 | 90 | Cr | 2a | 0.000 | 0.000 | 0.000 |
| Cubic 229 | | | | | | | C/N/O | 6b (oct) | 0.000 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 12d (tet) | 0.250 | 0.000 | 0.500 |
| Fe ($Im\bar{3}m$) | 2.833 | 2.833 | 2.833 | 90 | 90 | 90 | Fe | 2a | 0.000 | 0.000 | 0.000 |
| Cubic 229 | | | | | | | C/N/O | 6b (oct) | 0.000 | 0.500 | 0.500 |
| | | | | | | | C/N/O | 12d (tet) | 0.250 | 0.000 | 0.500 |