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FIRST-WALL-COATING CANDIDATES FOR ICF REACTOR
CHAMBERS USING DRY-WALL PROTECTION ONLY(a)

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ABSTRACT

Twenty pure metals were considered as potential candidates for first-wall coatings of ICF reactor chambers. Seven were found to merit further consideration based on the results of computer-code calculations of figures-of-merit. The seven are rhenium, iridium, molybdenum, chromium, tungsten, tantalum, and niobium (listed in order of decreasing values of figures-of-merit). The calculations are based on mechanical, thermal, and vacuum vaporization engineering constraints. A number of alloys of these seven metals are suggested as additional candidates.

INTRODUCTION

The engineering solutions to the protection of the first solid surface of ICF (Inertial Confinement Fusion) reactor chambers include the potential applications of flowing liquid metals, thin liquid metal films, high density gases, magnetic fields, and thin metallic coatings, as well as various combinations of each of these schemes. Only the scheme with metallic coatings uses another solid material to protect the chamber structural wall. Such coatings must simultaneously satisfy mechanical, thermal, and vacuum vaporization engineering constraints during reactor operation, and these constraints seriously limit the number of materials to be considered. If these constraints are then coupled to considerations of manufacturability, coating technology development, and irradiation damage at elevated temperatures under pulsed loadings, the potential candidates for first wall coatings will more than likely be restricted to a mere handful of materials. The following is the result of a brief study to initiate a selection process for establishing coating candidates. The study is limited to considering mechanical, thermal, and vacuum vaporization engineering constraints as they apply to pure metals. Considerations of cost, fabrication, radiation effects, and material compatibility were not

included in this initial effort. The establishment of a set of algorithms for compilation of physical data and figures-of-merit was achieved. A code based on the algorithms was created and used to generate a ranking of candidates for first wall coatings.

COATING CANDIDATE SELECTION AND RANKING METHOD

The method developed in this study to allow materials to be selected and ranked is based on the development of a computer code. The code is used as a data bank for physical properties of materials and as a relatively simple tool for rank ordering these materials. The rank ordering is accomplished by a set of relatively simple algorithms to obtain numerical values for figures-of-merit (FOM) which not only account for material properties, but also for features of the reactor cavity and the pulsed energy produced by the pellet explosions. The algorithms and code have been developed in a manner which permits additional materials, material properties, and/or FOM to be incorporated at a later time.

The version of the code, which has been named CANDID (short for CANDIDATE DATA AND RANKING), developed for this study has data for twenty pure metals. The data incorporated for each candidate consists of fourteen physical and mechanical properties which are either temperature independent, very weakly dependent on temperature, or values at room temperature (20-25°C). There are also five more physical and mechanical properties incorporated which are treated as temperature dependent and the FOM values are calculated accordingly. Tables 1 and 2 are examples of the set of properties collected^{1,2,3} for this study and printed as output from CANDID.

The FOM calculations are based on estimating a number of first wall parameters related to the operation of the device and the coating material properties. These parameters are converted into a set of dimensionless variables ranging from

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zero to unity where the higher the value, the higher the potential merit of the material. This set is then combined into a single FOM per material by taking a weighted sum of these normalized values. The weights are established by selecting the relative importance of each individual term. Since there is no obvious means of setting weights, a number of weighting schemes were used.

There are six independence FOM parameters selected for this study based on the following parameters:

1. The maximum temperature rise at the coating surface due to the energy pulse. This parameter indicates the design margin in maintaining the coating below melting conditions.

TABLE 1

PHYSICAL PROPERTIES OF IRIIDIUM, MOLYBDENUM, RHEINIUM, TANTALUM, AND TUNGSTEN

ATOMIC SYMBOL	Ir	Mo	Re	Ta	W
ATOMIC MASS (u)	192.9	95.9	186.2	180.9	183.9
STRUCTURE (1=FCC, 2=BCC, 3=CPH)	FCC	BCC	FCC	BCC	BCC
LATTICE CONSTANT (nm)	-	.31468	.27600	.33026	.31652
DENSITY (g/cm ³) at 20-25°C	22.65	10.22	21.04	16.60	19.25
MELTING TEMPERATURE (K)	2720	2883	3453	3269	3683
TH. NEUTRON CROSS SECTION (b)	-	-	-	21	-
LAT. HEAT OF VAPOR. (kJ/kg)	-	5123	-	4215	-
ENTROPY (J kg ⁻¹ K ⁻¹)	190	300	225	229	182
VAPOR PRESSURE AT MELTING (torr)	0.065	0.014	0.053	0.0096	0.037
EVAPORATION (g cm ⁻² S ⁻¹)	1.0x10 ⁻³	1.5x10 ⁻⁴	7.1x10 ⁻⁴	1.3x10 ⁻⁴	4.8x10 ⁻⁴
POISSONS RATIO AT 20°C	0.26	0.32	0.49	0.35	0.29
SHEAR MODULUS AT 20°C (GPa)	205	147	154	69	160
TENSILE STRENGTH (MPa)	1170	775	1160	200	350
HARDNESS (HV)	22	100	270	100	100
TEMPERATURE DEPENDENT DATA AT 20°C					
CONDUCTIVITY (W m ⁻¹ K ⁻¹)	147	142	71	54	160
SPECIFIC HEAT (J kg ⁻¹ K ⁻¹)	130	276	146	139	136
EXPANSION COEF. (10 ⁻⁶ m/m K ⁻¹)	6.8	1.6	10.0	6.5	3.4
TENSILE MODULUS (GPa)	517	320	460	186	410
YIELD STRENGTH (MPa)	234	400	930	180	150

TABLE 2

TEMPERATURE DEPENDENT PROPERTIES FOR IRIIDIUM, MOLYBDENUM, TANTALUM, AND TUNGSTEN

ATOMIC SYMBOL	Ir	Mo	Ta	W
DATA AT 500°C				
CONDUCTIVITY (W m ⁻¹ K ⁻¹)	110	132	66	130
SPECIFIC HEAT (J kg ⁻¹ K ⁻¹)	142	276	153	143
EXPANSION COEF. (10 ⁻⁶ m/m K ⁻¹)	7.2	2.8	6.7	4.8
TENSILE MODULUS (GPa)	465	302	168	390
YIELD STRENGTH (MPa)	234	150	50	125
DATA AT 1000°C				
CONDUCTIVITY (W m ⁻¹ K ⁻¹)	74	111	78	120
SPECIFIC HEAT (J kg ⁻¹ K ⁻¹)	159	285	164	152
EXPANSION COEF. (10 ⁻⁶ m/m K ⁻¹)	7.8	3.9	7.0	5.7
TENSILE MODULUS (GPa)	414	250	150	365
YIELD STRENGTH (MPa)	43	100	38	75

2. The bulk temperature rise in the coating layer due to the deposition of energy from a single pulse. The bulk temperature rise for this design should be minimized so as to reduce the stresses at the bond between the structural wall and the coating.

3. The material frequency associated with the first wall due to the pulsed energy load. Any mismatch in frequencies between the coating and structural wall will result in the weakening of the bond due to the induced tensile forces set up by the vibrational motions.

4. The maximum first-cycle strain in the coating layer due to the motion of the cavity wall. This parameter represents the mechanical strains induced by the motion of the wall independent of any thermal effects and should be minimized.

5. The thermal stress in the coating layer, due to the temperature gradient. The thermal stress levels relative to the yield strength of the coating indicates the integrity of the material to remain attached to the wall.

6. The evaporation rate of coating material at/near the melting temperature. This parameter indicates the ease with which it is possible to remove pellet material which has accumulated on the wall as the device is pulsed.

The six parameters indicated above are calculated using the following expressions:

1. Maximum temperature rise, ΔT_m .

$$\Delta T_m = \frac{H_W}{S_A} \left(\frac{\pi}{4} \tau_p k_p \rho C_p \right)^{-1/2}$$

where H_W is the total first wall heat load, S_A is the first wall area, k is the thermal conductivity, ρ is the mass density, C_p is the specific heat, and τ_p is the pulse length of the heat load.

2. Bulk temperature rise, ΔT_B .

$$\Delta T_B = H_W / (S_A h \rho C_p)$$

where h is the thickness of the coating layer.

3. Natural frequency of material x , ω_x .

$$\omega_x^2 = 2 E_x / (\rho_x R_o^2 (1 - \nu_x))$$

where E_x is the tensile modulus, R_o is the cavity radius, and ν_x is Poisson's ratio.

4. Maximum first-cycle strain, ϵ_m .

$$\epsilon_m = ((1 - \nu_s) / (2 \rho_s E_s)) \times (I_r / h_s)$$

where the subscript s refers to the first wall structural material, and I_r is the reflected pressure impulse to the microexplosion, and⁴

$$I_r = E_{DT}^{0.8} (2 R_o)^{-1.39}$$

E_{DT} is the total fusion energy per pulse, and R_o is the cavity radius.

5. The thermal stress in material x , S_x .

$$S_x = 0.5 \alpha_x E_x \Delta T / (2(1 - \nu_x))$$

where α is the linear expansion coefficient, and ΔT is the temperature drop expected across the coating layer.

6. The evaporation rate, $\dot{m}_E$, at temperature T ,

$$\dot{m}_E = P_v S_A (A/T)^{1/2}$$

where P_v is the vapor pressure, A is the atomic mass of the coating material, and the values of P_v are calculated using the following expression

$$\log P_v = A - \frac{B}{T}$$

for which the constants A and B are given in Reference 2.

In the conversion of these parameters to dimensionless magnitudes ranging from 0 to 1, each parameter was divided by an appropriate upper limit. This ratio was either used directly or subtracted from unity so that the final value was close to unity if meritorious or close to zero if not meritorious. For example, the maximum temperature rise was divided by the difference between the melting temperature T_m and the operating temperature T_o , and then subtracted from one, i.e.,

$$FOM(1) = 1 - \frac{\Delta T_B}{T_m - T_o}$$

where $FOM(1)$ is set to zero if $\Delta T_m > (T_m - T_o)$. As another example,

$$FOM(4) = 1 - \frac{Y_{MOD}}{1 - \frac{c}{Y_c}} \frac{c}{Y_c}$$

where Y_c is the yield strength of the coating material and Y_{MOD} tensile modulus of the coating material.

An overall figure-of-merit, $FOM(7)$, is assumed to be a weighted average of the above six FOM, where

$$FOM(7) = \frac{1}{6} \sum_{i=1}^6 FOM(i)$$

and

$$I = \frac{1}{6} \sum_{i=1}^6 W_i$$

For this first application of CANDID, a number of sets of W_i values were used.

RESULTING FIGURES-OF-MERIT VALUES

The CANDID code was used to obtain the component FOM values for the 20 candidate materials. The results are shown in Table 3 for these materials which are all pure metals. Zeros indicate a failure of the material, e.g., aluminum melted since $FOM(1) = 0.0$. Failure $FOM(2)$ indicated the bulk material rises more than 10% of the operating value of 773K assumed for the first wall. If $FOM(4) = 0$, the "cold" stress due to mechanical motion exceeds the yield strength, and if $FOM(5) = 0$ the thermal stress due to a temperature gradient of 50K exceeds the yield strength. The assumptions associated with the operation of the ICF reactor are summarized in Table 4. To evaluate $FOM(6)$ an arbitrary value of 1 gram was chosen for the mass of each pellet. This value was chosen to permit $FOM(6)$ to vary over the full range from near zero to unity for the 20 materials.

Composition FOM values and ranking for each of four weighting schemes as well as the average for all four were calculated. Aluminum, silver, copper, and vanadium ranked uniformly low, while

TABLE 3
COMPONENT FIGURES-OF-MERIT VALUES (V) AND RANKINGS (R)

Material	FOM(1)		FOM(2)		FOM(3)		FOM(4)		FOM(5)		FOM(6)	
	V	R	V	R	V	R	V	R	V	R	V	R
Al, Aluminum	0	11	.32	15	.99	2	.15	18	0	17	0	20
Ag, Silver	0	11	.33	14	.75	17	.57	13	0	17	.07	11
Au, Gold	0	11	.33	13	.60	20	.89	2	.81	6	0	17
Be, Beryllium	.12	9	.53	2	.61	19	.72	10	.44	15	.26	7
Cr, Chromium	.13	8	.50	5	.93	8	.54	14	.66	13	1.00	1
Cu, Copper	.18	6	.52	3	.92	11	0	19	0	17	.01	15
Fe, Iron	0	11	.51	4	.98	6	.80	5	.71	9	.54	5
Ir, Iridium	.56	3	.44	9	1.00	1	.38	15	.49	14	1.00	1
Mo, Molybdenum	.58	2	.42	11	.90	12	.75	7	.95	1	.19	8
Nb, Niobium	.17	7	.29	16	.88	13	.83	4	.85	4	.02	14
Ni, Nickel	0	11	.61	1	.98	5	0	19	0	17	.09	10
Pt, Platinum	.01	10	.42	10	.76	16	.72	9	.70	11	.01	16
Re, Rhenium	.55	4	.46	6	.92	9	.80	6	.84	5	.90	3
Si, Silicon	0	11	0	19	.80	15	.73	8	.91	3	.02	13
Ta, Tantalum	.36	5	.29	17	.85	14	.69	12	.74	8	.16	9
Th, Thorium	0	11	0	19	.69	18	.86	3	.80	7	0	18
Ti, Titanium	0	11	.45	8	.92	10	.71	11	.71	10	.07	12
V, Vanadium	0	11	.46	7	.99	3	.24	16	.12	16	.32	6
W, Tungsten	.70	1	.37	12	.99	4	.20	17	.67	12	.60	4
Zr, Zirconium	0	11	.13	18	.93	7	.91	1	.94	2	0	19

TABLE 4

CANDID INPUT DATA FOR THE ICF DEVICE
AND STRUCTURAL FIRST WALL

RO, ICF REACTOR CHAMBER RADIUS (m)	10.00
HO, CHAMBER WALL THICKNESS (m)	.0200
H, 1ST WALL COATING THICKNESS (m)	.0010
TO, 1ST WALL OPERATING TEMP. (K)	773.00
EOT, ENERGY PER PELLET EXPLOSION (MJ)	350.00
RATE, DROP RATE OF PELLETS (Hz)	10.00
PMASS, PELLET MASS (g)	1.0000
WLOAD, HEAT LOAD TO COATING (MJ)	160.00
GTEM, CAVITY GAS TEMPERATURE (K)	832.00
FATM, FRACT ABOVE TM FOR MELTING	.0200
PLEN, ENERGY PULSE LENGTH (s)	6.500E-05
GPRES, CAVITY GAS PRESSURE (torr)	1.000E-04
RHOC, DENSITY OF WALL MATL (gm cm ⁻³)	7.70
POISC, POIS RATIO FOR WALL MATL	.2650
YMOCC, YOUNGS MODULUS OF WALL (GPa)	175.00
YOC, YIELD STRENGTH OF WALL (MPa)	340.00
TDROP, TEMP DROP ACROSS COATING (K)	50.00
TDMAX, TEMP DROP MAX RELATIVE TO TO	.1000
TCOCC, T. COND. OF WALL (W M ⁻¹ K ⁻¹)	29.00
CPC, SP. HEAT OF WALL (J kg ⁻¹ K ⁻¹)	725.00
ALPHAC, WALL EXPANSION (10 ⁻⁶ K ⁻¹)	11.30
STO, WALL TENSILE ST. (MPa)	480.00
RPIC, REF. PRES. IMP. CONST.	150.00

rhodium, molybdenum, and chromium ranked uniformly high. Iridium and tungsten ranked high in all, but the FOM which emphasizes the mechanical characteristics. The candidate selected in previous studies, tantalum, was found to be ranked at a consistent seventh place.

Of the 20 candidate materials investigated, 11 were found to have zero FOM values in one or more of the component FOM. Aluminum, silver, gold, copper, nickel, silicon, thorium, and zirconium have two or more zeros and were dropped as potential first wall coating candidates. The three materials, iron, titanium, and vanadium, have one zero value each and were also dropped. Note that although iron has a zero FOM component, the remaining values permitted the material to achieve high scores overall. Because beryllium is such a low-Z material it was also excluded. Even though platinum has no zeros, it has an overall ranking which is low and has a near zero FOM(1) value, and it was not included in the final selection.

The materials, associated atomic charge, melting point, and FOM value which remain as candidates are, in order of FOM ranking:

- A. Re, Z = 186, $T_m = 3453$ K, FOM = .76
- B. Ir, Z = 193, $T_m = 2720$ K, FOM = .63
- C. Mo, Z = 96, $T_m = 2883$ K, FOM = .63
- D. Cr, Z = 52, $T_m = 2148$ K, FOM = .61

- E. W, Z = 184, $T_m = 3683$ K, FOM = .57
- F. Ta, Z = 181, $T_m = 3269$ K, FOM = .50
- G. Nb, Z = 93, $T_m = 2741$ K, FOM = .49

The lowest FOM is for aluminum and has a value of 0.16. Copper and nickel were next with 0.18.

Based on the requirement of a high-Z material and a high melting point, chromium would likely be the first to be dropped when further studies are made, but since chromium is one of the more common materials relative to the list of seven candidates, it may have many merits worth considering. Four of the candidates have very high Z-values as well as high T_m -values, but due to material availability and manufacturability, all four may not represent viable candidates. The remaining materials, molybdenum and niobium, are only moderately-high-Z materials making them of limited value in terms of pellet materials. For only five of the seven metals listed above was there sufficient data on the temperature dependence of physical and mechanical properties to permit the calculation of FOM values at elevated temperatures. Values at room temperature, 500°C, and 1000°C are shown in Table 5. In all cases the values decrease with increasing temperature with a character differing for each metal. Above 1000°C all five materials have zero values for component FOM.

For a number of the above pure metal candidates, problems in manufacturability or loss of ductility could eliminate their applicability. As a potential means of reducing such problems so that such candidates remain attractive, alloys with the candidate pure metal as a base should be considered. The following is a list of alloys which could be considered:

- A. Mo-Re and W-Re
- B. Pt-Ir
- C. Mo-W, Mo-Ti, and TiZr
- D. W-Ni-Cu and W-Ni-Fe
- E. Ta-W and Ta-Hf
- F. Nb-Zr and Nb-W-Zr

TABLE 5

OVERALL FIGURES-OF-MERIT VALUES VS.
TEMPERATURE FOR FIVE CANDIDATES

Candidate	~20°C	500°C	1000°C
	~300K	773K	1273K
Mo, Molybdenum	.63	.52	.49
Nb, Niobium	.51	.50	.28
Ta, Tantalum	.51	.32	.31
W, Tungsten	.59	.54	.45
Ir, Iridium	.64	.66	.49

Both rhenium and iridium are scarce and thus very costly, and the most likely use for either metal may lie in the addition of small amounts to materials such as molybdenum, tungsten, chromium, and platinum.

SUMMARY AND RECOMMENDATIONS

Using the CANDID code, 20 pure metals were investigated for potential application as first wall coatings for ICF reactor chambers. The data base of material properties included 19 physical parameters for each of the 20 candidate metals. Based on a number of these parameters as well as on several key ICF device parameters, six figures-of-merit (FOM) were calculated using CANDID for each candidate. By taking weighted sums of the six FOM values, overall FOM values were obtained. The six FOM calculations are based on mechanical, thermal, and vacuum vaporization engineering constraints. The 20 pure metal candidates investigated were aluminum, silver, gold, beryllium, chromium, copper, iron, iridium, molybdenum, niobium, nickel, platinum, rhenium, silicon, tantalum, thorium, titanium, vanadium, tungsten, and zirconium.

The candidate materials recommended for further consideration as first wall coatings are

Rhenium (Re)	Iridium (Ir)
Molybdenum (Mo)	Chromium (Cr)
Tungsten (W)	Tantalum (Ta)
Niobium (Nb)	

where the list is in rank order based on FOM values. Tantalum is the material previously selected⁵ for the ICF dry wall design.⁶ Based on the relative rankings of these seven materials in each of the six areas where FOM values were calculated the following observations are made:

- A. W and Mo are especially suited as resisting surface melting having the highest values for FOM(1).
- B. Cr and Re are excellent candidates for maintaining small temperature changes at the interface with the structure wall.
- C. Ir and W are the most compatible of the seven in terms of matching the natural frequency of the structural wall.
- D. Re, Mo, and Nb are the best candidates in terms of withstanding both mechanical and thermal loads (FOM(4) and FOM(5)).
- E. Ir and Cr are particularly suited for wall conditioning by evaporation at elevated temperatures (FOM(6)).

Some basic weaknesses in the properties of the seven candidates include:

- A. Low FOM in performance under pulsed loading for Ir, Cr, and W.
- B. Low FOM in the matching of natural frequencies with that of the structural wall for Ta and Nb.
- C. Low FOM in bulk temperature rises for Ta and Nb.
- D. Low evaporation rates at elevated temperatures for Nb.

Overall, rhenium has component FOM values which are relatively high in all areas investigated. Molybdenum has FOM values which are good to very good in all areas and has no areas with low FOM values. All the other candidates show weaknesses in one or more of the areas examined. The candidate selected for the ICF dry wall study, i.e., tantalum, continues to show promise, but there are areas of potential weakness in that three of the six FOM values placed Ta in the lower half of the ranking when considering all 20 candidates. Since the six FOM chosen to characterize the candidate metals are limited to thermal, mechanical, and vacuum considerations, it is recommended that additional FOM be selected and used in future work. These could include cost, fabrication, irradiation effects, compatibility with pellet design, etc.

In collecting temperature-dependent data for this study and for CANDID input, very little high temperature data was found. For five candidates (Mo, Nb, Ta, W, and Ir) enough data was collected to permit a limited temperature-dependent study. The FOM values were found to be strong functions of temperature, and were found to have changes with temperature which do not follow any characteristic pattern for the five materials studied. At the highest temperature (1273 K) all FOM values were much lower than at 20°C, indicating the importance of using data at the elevated temperatures expected in the ICF reactor.

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