Short Note

Relationship Between the Mechanical Properties of an Irradiated Metal Alloy and the Mechanical Properties of the Irradiated Elements of the Alloy

Valeriy Kizka *

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Relationship between the Mechanical Properties of an Irradiated Metal Alloy and the Mechanical Properties of the Irradiated Elements of the Alloy

V. A. Kizka

Department of experimental nuclear physics, V. N. Karazin Kharkiv National University, Kharkiv, Ukraine; valeriy.kizka@karazin.ua

Abstract: In the article, we are trying to find a general law that describes the physical properties of a complex compound through the same physical properties of compound elements. For metal alloys operated under extreme conditions - neutron and proton irradiations and thermal heating, the mechanical properties of these alloys and their elements have been studied. It turned out that the ultimate tensile strength of tantalum alloys used in the design of space reactors can be expressed in terms of the weighted sum of the ultimate tensile strengths of its elements in the range of neutron doses: (0 ÷ 0.96) displacement per atom (dpa) for Ta–10W alloy and (1.4 ÷ 1.7) dpa for T–111 alloy with a neutron energy of more than 0.1 MeV. For tungsten binary alloys used in the design of fusion reactors, the Vickers hardness can also be expressed in terms of the weighted sum of the Vickers hardnesses of the alloy elements in the range of proton irradiation doses: (0 ÷ 0.05) dpa for W-1%Re alloy, (0.05 ÷ 0.2) dpa for W-3%Re alloy and (0.05 ÷ 1) dpa for W-1%Ta with a proton energy of 1 MeV.

Keywords: Tantalum alloys; Tungsten binary alloys; Irradiation; Neutron irradiation; Proton irradiation; Yield strength; Ultimate tensile strength

From our previous results regarding thermal conductivity [1,2] and melting/solidification temperature [3] of nuclear fuel fragments, oxide nuclear fuel and other nuclear ceramics, we concluded that for an arbitrary material, we can express its arbitrary physical property through atomic weighted or mass weighted sum of the corresponding physical properties of the elements of this material. This conclusion is also confirmed by the result on the superconductivity transition temperatures of high-temperature Y- and Hg-cuprates [4]. We have shown that in limited ranges of temperatures [1,2] or mole fractions of mixtures of actinide oxides [3], such weighted sums are multiplied by a constant. In other ranges of temperatures or mole fractions, we describe the physical properties of nuclear materials in terms of a weighted sum multiplied by a variable that changes according to the change in lattice parameters with mole fractions of the elements or temperature [3].

In this paper, we also describe the mechanical properties of metal alloys in terms of the mass-weighted sum of the mechanical properties of the alloy elements, multiplied by a constant in certain ranges of irradiation doses. We cannot conclude how to describe the mechanical properties of these alloys in other ranges of irradiation doses, since we did not find data on the behavior of their lattice parameters with a change in the irradiation dose.

If we consider an arbitrary solid body represented as a chemical compound, or a mechanical mixture, or a solid solution $A_nB_mC_k\ldots$, then the best formula for describing an arbitrary physical property $L_{AnBmCk\ldots}$ of this solid body through the physical properties of its elements is the following:

$$\frac{1}{L_{A_nB_mC_k\ldots}(\Omega)}=\frac{1}{(n\cdot L_A(\Omega)+m\cdot L_B(\Omega)+k\cdot L_C(\Omega)+\ldots)}\cdot\left[\frac{1}{n\cdot A}+\frac{1}{m\cdot B}+\ldots+\frac{h(\Omega)}{k\cdot C}\right], \qquad (1)$$

where $L_A(\Omega)$ is a physical property of element A, etc., A is the atomic number of element A and so on. Ω is a set of external and internal parameters of the medium and the solid, respectively – temperature *T*, pressure *p*, radiation *D*, impurity concentration *x* or some elements of this solid, and so on: $\Omega = \{T, p, D, x, \ldots\}$, where $T, p, D, x, \ldots \in \mathbf{R}$ (set of real numbers). $h(\Omega)$ is a structural parameter depending on the dependence of the lattice parameters of $A_nB_mC_k\ldots$ on the elements Ω and $h \in Q$ (set of rational numbers) [1–3]. $h(\Omega)$ is associated in (1) with the most electronegative element, in our case it is the symbol C. Presence of the atomic numbers of all elements of the given complex compound is necessary because charges of nuclei define electronic structure of the solid body.

It turned out that for some $\Omega' \subset \Omega$ the structure parameter h is a constant: $h(\Omega') \equiv h$ [1], [2], [3]. In this case the physical observable $L_{A_nB_mC_k\ldots}(\Omega')$ can be represented in the next form:

$$L_{A_nB_mC_k\ldots}(\Omega') = (n\cdot L_A(\Omega') + m\cdot L_B(\Omega') + k\cdot L_C(\Omega') + \ldots)\cdot b,$$

$$where\ \ b = \left[\frac{1}{n\cdot A} + \frac{1}{m\cdot B} + \ldots + \frac{h}{k\cdot C}\right]^{-1}, \qquad (2)$$

and $\Omega' = \{T', p', D', x', \ldots\}$, where $T' \in [T_1 \div T_2]$ (some temperature range) and so on.

Consider a set of tantalum alloys used in the construction of space reactors. The first is the T–111 alloy with the following content (wt%) of elements: Ta- balk, Hf – 2%, W – 8.5% [5]. Samples T–111 were irradiated with fast neutrons with energy E > 0.1 MeV with doses of [0 ÷ 1.7] dpa and irradiation temperatures of [723 – 923] K (Table 2) [5]. Mechanical tests when measuring the yield strength $\sigma_{0.2}$ and ultimate tensile strength σ_t of these samples were carried out at the same temperatures: $T_{irrad} = T_{test}$. To apply formula (1), it is necessary to know the same mechanical values for all elements of the alloy (Ta, Hf and W) in the same radiation doses and temperature ranges as for the alloy. The authors of [5] found this out only for the Ta solvent. For monocrystalline and polycrystalline samples of tungsten W, we found the necessary data in [6]. But in [6], the data obtained using proton irradiation at higher doses (Table 1) and lower T_{irr} are given. Mechanical tests of samples W were carried out at room temperature RT (Table 1). In any case, we used these data when calculating according to formula (1), since we did not find another alternative.

Formula (1) for T-111 has the following form:

$$\frac{1}{\sigma_{0.2_{T-111}}(\Omega_{T-111})} = \frac{1}{0.895\cdot\sigma_{0.2_{Ta}}(\Omega_{Ta}) + 0.085\cdot\sigma_{0.2_W}(\Omega_W)}\left[\frac{1}{0.895\cdot Ta} + \frac{1}{0.02\cdot Hf} + \frac{h(\Omega_{T-111})}{0.085\cdot W}\right], \qquad (1.1)$$

where atomic numbers: Ta = 73, Hf = 72, W = 74. The electronegativities X of these elements are as follows: $X_{Ta} = 1.5$ [7], $X_{Hf} = 1.3$ [7], $X_W = 2.36$ [8]. Therefore W is related to h in (1.1). The set of parameters $\Omega_{material} = \{D, T_{irr}, T_{test}\}_{material}$ is associated with a specific material and their values for its elements are presented in Tables 1 and 2.

Table 1. Mechanical properties and conditions of irradiation of W-samples irradiated with protons with an energy of 580 MeV and unirradiated W-samples, irradiated with neutrons with energy E > 0.1 MeV and unirradiated Ta-samples, and tested for strength at room temperature RT: yield strength $\sigma_{0.2}$, ultimate tensile strength σ_t. Data taken from [5] for Ta and from [6] for W.

Material	T_{irrad}(°K)	Dose (dpa)	$\sigma_{0.2}$(MPa)	σ_t(Mpa)
$W_{monocrystal}$	300	0	417	464.5
	405	10.2	670	685
$W_{polycrystal}$	300	0	broken	555.3
	408	10.2	broken	268
Ta	728	0	78.25	246.5
	853	0	61.8	214
	703	0.96	465	536
	753	1.4	620	689
	853	1.7	514	551

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Table 2. Mechanical properties and conditions of neutron irradiation with neutron energy E > 0.1 MeV of irradiated and non-irradiated Ta alloys. The experimental data were taken from [5], the theoretical values were obtained according to (1.1) – (1.3). Fitting parameters h are also shown. Relative errors δ are also shown, they are calculated by the formula: $\delta = |1 - \sigma_{theory}/\sigma_{experiment}| \cdot 100\%$. The use of data for polycrystalline or monocrystalline W in calculations is also displayed in the column headings for theoretical σ_t. Here $T_{test} = T_{irr}$.

Material	Dose (dpa)	T_{irr} [°K]	$\sigma_{0.2}$(Mpa) experiment	σ_t(Mpa) experiment	h, $\sigma_{0.2}$(Mpa) (δ%) theory	h, σ_t(Mpa) (δ%) theory, monocrystal	h, σ_t(Mpa) (δ%) theory, polycrystal
T–111	0	723	569	628.5	$h = -3.3$, 569.8(0.1%)	$h = -1.86$, 628.2(0.05%)	$h = -1.78$, 627.6(0.1%)
		833	486	552.7	$h = -3.3$, 490.3(0.9%)	$h = -1.86$, 557.9(0.9%)	$h = -1.78$, 559.4(1.2%)
	0.78	723	1370	1370	$h = -2.3$, 1375(0.4%)	$h = -2.0$, 1373(0.2%)	$h = -2.2$, 1395.9(1.9%)
	1.4	803	1370	1370	$h = -1.7$, 1392.2(1.6%)	$h = -1.4$, 1385.3(1.1%)	$h = -1.49$, 1352.2(1.3%)
	1.7	923	1050	1070	$h = -1.4$, 1061.2(1.1%)	$h = -1.2$, 1062.4(0.7%)	$h = -1.49$, 1091(2.0%)
ASTAR–811C	0	763	710	855	$h = -14.4$, 720.6(1.5%)	$h = -13.42$, 845.1(1.2%)	$h = -13.4$, 860.2(0.6%)
		873	586	745	$h = -14.43$, 579.2(1.2%)	$h = -13.42$, 750.1(0.7%)	$h = -13.34$, 742.4(0.3%)
	1.1	763	1385	1425	$h = -13.2$, 1376(0.6%)	$h = -13$, 1427.8(0.2%)	$h = -13.13$, 1417.6(0.5%)
	1.7	873	1230	1270	$h = -12.71$, 1217.1(1.0%)	$h = -12.65$, 1268.6(0.1%)	$h = -12.8$, 1261.7(0.6%)
Ta–10W	0	728	486	564	$h = 1.65$, 482.4(0.7%)	$h = 3.5$, 561.1(0.5%)	$h = 3.6$, 564.8(0.1%)
		803	447	521	$h = 1.56$, 441.7(1.4%)	$h = 3.4$, 514.4(1.3%)	$h = 3.5$, 519.5(0.3%)
	0.96	703	1020	1030	$h = 3.5$, 1014.5(0.5%)	$h = 3.9$, 1036.2(0.6%)	$h = 3.6$, 1033.4(0.3%)
	1.4	753	989.5	989.5	$h = 4.7$, 979.9(1.0%)	$h = 5.2$, 977.9(1.2%)	$h = 4.8$, 992.1(0.3%)

To calculate the ultimate tensile strength, it is necessary to replace $\sigma_{0.2}$ with σ_t in formula (1.1). The result of using formula (1.1) is presented in Table 2. Since the parameters in the set Ω vary when moving from material to its elements, the mechanical values of the elements for calculation according to (1.1) were taken with the closest values of irradiation doses and temperatures. In the case of W, we only have a dose of 10.3 dpa. This is more than we need, but we took data for W at these irradiation doses, having no alternative. We neglected the influence of the mechanical properties of Hf in (1.1), but in any case there are no such data for irradiated Hf. From Table 2 it can be seen that in the absence of irradiation, the mechanical properties of T–111 can be expressed through (2) at fixed h for different T_{irr} and T_{test}. In the presence of radiation, only σ_t is expressed through (2) with data for polycrystalline W and $D_{T\text{-}111} = (1.4 - 1.7)$ dpa. Since we do not have data on the lattice parameters of T–111 at various temperatures and radiation doses, we cannot reveal the dependence of $h(\Omega)$ on the lattice parameters. Probably from [3] it should look like this: $h(\Omega) = g_1 \cdot \partial_D a + g_2 \cdot \partial_{Tirr} a + g_3 \cdot \partial_{Ttest} a$, where a is the lattice parameter, g_i are constants.

The next tantalum alloy is ASTAR–811C with the content (wt%): Ta-balk, Hf - 0.9%, Re - 1.39%, W - 8.2% [5]; the electronegativities: $X_{Ta} = 1.5$ [7], $X_{Hf} = 1.3$ [7], $X_W = 2.36$ [8], $X_{Re} = 1.9$ [7]. Formula (1) has the following form:

$$\frac{1}{\sigma_{0.2_{ASTAR}}(\Omega_{ASTAR})}=\frac{1}{0.8951\cdot\sigma_{0.2_{Ta}}(\Omega_{Ta})+0.082\cdot\sigma_{0.2_{W}}(\Omega_{W})}\left[\frac{1}{0.8951\cdot Ta}+\frac{1}{0.009\cdot Hf}+\frac{1}{0.0139\cdot \mathrm{Re}}+\frac{h(\Omega_{ASTAR})}{0.082\cdot W}\right], \qquad (1.2)$$

where atomic nymbers: Ta = 73, Hf = 72, W = 74, Re = 75. For ultimate tensile strength, it is necessary to change $\sigma_{0.2}$ to σ_t in (1.2). We neglected the influence of $\sigma_{0.2}$ and σ_t for Hf and Re on the calculation results, in any case we did not find the necessary data for these elements. It can be seen from Table 2 that only for zero radiation it is possible to express $\sigma_{0.2}$ for the ASTAR–811C alloy in the form (2) with a constant h as T_{irr} changes and with data for monocrystalline W. The behavior of $h(\Omega)$ with a change in the irradiation dose is difficult to describe unless data on the lattice parameters are available.

Two more words about ASTAR–811C. It contains 0.025% of carbon [5]. Taking the data for carbon in the state of diamond $\sigma_{0.2}$ = 40 GPa [9], the product 0.00025·40 GPa gives a contribution comparable to the term for W in the weighted sum in (1.2). But we neglected this, although carbon has a decisive influence on the mechanical properties of this alloy, forming microstructural objects in the alloy [5]. Probably, this neglect leads to the absence of the constant h at different doses D for the ASTAR-811C data in Table 2. But again, we did not find suitable data for the irradiated diamond.

The last tantalum alloy is Ta–10W with the content (wt%): Ta- balk, W - 10.2% [5]. Formula (1) has the following form:

$$\frac{1}{\sigma_{0.2_{Ta-10W}}(\Omega_{Ta-10W})}=\frac{1}{0.898\cdot\sigma_{0.2_{Ta}}(\Omega_{Ta})+0.102\cdot\sigma_{0.2_{W}}(\Omega_{W})}\left[\frac{1}{0.898\cdot Ta}+\frac{h(\Omega_{Ta-10W})}{0.102\cdot W}\right], \qquad (1.3)$$

where again we need to change $\sigma_{0.2}$ to σ_t for ultimate tensile strength calculations. The calculation data are given in Table 2. From Table 2 it can be seen that with an irradiation dose in the range (0 ÷ 0.96) dpa and irradiation and mechanical testing temperatures close to 700 K, the ultimate tensile strength of the Ta–10W alloy is described by the expression (2) where h is a constant value. There is no data for lattice parameters changing with dose radiation and temperatures of irradiation and mechanical test.

We have considered binary W alloys studied under proton irradiation in the dose range (0 ÷ 1) dpa and with proton energy E = 1 MeV [10]. Temperature of irradiation 800°C, Vickers hardness H_V test was carried out at room temperature. The authors of [10] studied pure tungsten under the same conditions as alloys (Table 3). Formula (1) for W-1%Re and W-3%Re alloys is as follows:

$$\frac{1}{H_{V_{W-wt\%Re}}(\Omega_{W-wt\%Re})}=\frac{1}{(1-wt)\cdot H_{V_{W-wt\%Re}}(\Omega_{W})}\cdot\left[\frac{1}{wt\cdot \mathrm{Re}}+\frac{h(\Omega_{W-wt\%Re})}{(1-wt)\cdot W}\right], \qquad (1.4)$$

where W = 74, Re = 75, wt = 0.01 for W-1%Re or 0.03 for W-3%Re. We neglected the Vickers hardness for Re due to the lack of relevant data for this element. Table 3 shows that HV for W-1%Re and W-3%Re alloys can be described by formula (2) in the dose ranges (0 ÷ 0.05) dpa and (0.05 ÷ 0.2) dpa, respectively. There are no data on the change in lattice parameters during irradiation for these alloys to clarify the form of $h(\Omega)$.

Table 3. Vickers hardness Hv of semples of tungsten alloys at various irradiation doses with protons with an energy 1 MeV at an irradiation temperature of 800°C. Experimental data are taken from [10]. The relative error δ is also shown, it is calculated by the formula: $\delta = |1 - Hv_{theory}/Hv_{experiment}|\cdot 100\%$. .

Dose (dpa)	Hv[HV] of pure W, experiment	Hv[HV] of W-1%Re, experiment	h, Hv[HV] (δ%) of W-1%Re, theory	Hv[HV] of W-3%Re, experiment	h, Hv[HV] (δ%) of W-3%Re, theory	Hv[HV] of W-1%Ta, experiment	h, Hv[HV] (δ%) of W-1%Ta, theory	Hv[HV] of W-3%Ta, experiment	h, Hv[HV] (δ%) of W-3%Ta, theory
0	408	369	**h = –18, 371.4(0.6%)**	365	h = 45, 369.4(1.2%)	443	h = –34, 445.9(0.7%)	463	h = 29, 459.8(0.7%)
0.05	537	484	**h = –18, 488.8(1.0%)**	449	**h = 50, 456.5(1.7%)**	536	**h = –28, 538.3(0.4%)**	530	h = 38, 528.3(0.3%)
0.2	612	602	h = –24, 602.4(0.07%)	528	**h = 50, 520.3(1.5%)**	609	**h = –28, 613.5(0.7%)**	644	h = 33, 647.8(0.6%)
1	659	675	h = –27, 676.2(0.2%)	609	h = 45, 596.7(0.03%)	655	**h = –28, 660.6(0.8%)**	716	h = 31, 719.4(0.5%)

Formula (1) for W-1%Ta and W-3%Ta alloys is as follows:

$$\frac{1}{H_{V_{W-wt\%Ta}}(\Omega_{W-wt\%Ta})}=\frac{1}{(1-wt)\cdot H_{V_{W-wt\%Ta}}(\Omega_W)}\cdot\left[\frac{1}{wt\cdot Ta}+\frac{h(\Omega_{W-wt\%Ta})}{(1-wt)\cdot W}\right], \qquad (1.5)$$

where W = 74, Ta = 73, wt = 0.01 for W-1%Ta or 0.03 for W-3%Ta. We neglected the Vickers hardness of Ta due to the lack of relevant data for this element. The calculation results are given in Table 3. We see that for W-1%Ta in the dose range (0.05 ÷ 1) dpa, the structural parameter h is a constant, and therefore the Vickers hardness can be described by formula (2). There are no data on the change in lattice parameters during irradiation for these alloys to clarify the form of $h(\Omega)$.

As a result, we can conclude that the existence of ranges of radiation doses and temperatures within which the mechanical properties of various metal alloys can be described by a weighted sum of the mechanical properties of the alloy elements, multiplied by a constant, tells us that this is a manifestation of a general law that can similarly describe any physical property of a compound. In other ranges of radiation and temperatures, we can describe an arbitrary physical property of a complex compound as a weighted sum of the physical properties of the constituent elements, multiplied by a variable depending on the lattice parameters of the complex compound. Unfortunately, such a simple idea, understandable even intuitively, i.e. if you want to know the properties of a complex compound under some conditions, you need information about the properties of all the constituent elements of the compound under the same conditions, this simple idea is completely ignored by researchers at the present time.

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