Hydrogen and Electric Field affect to the Iron Impurities removal from the molten Zirconium

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Abstract: Hydrogen and iron diffusion factors in the molten zirconium have been calculated using molecular-dynamic (MD) model. Molecular dynamics method using micro-canonical (NVT) ensemble has been used to analyze Iron and Zirconium diffusion factor dependence on electric field intensity and Hydrogen presence in the Zirconium melt. Results obtained are compared to the literary data on impurity removal in plasma-arc zirconium melting at hydrogen presence as well as in electron-beam and vacuum-arc melting. The limiting stage of iron removal from the melt is established. Contribution of electric field to the Iron removal is estimated. We carried out systematization of D_H^{Me} data for Zr, Nb, and Ta. Arrhenius equations analysis for D_H^{Me} and its extrapolation to premelting zone taking into account Gorsky – effect was carried out too. The analysis enabled to estimate D_H^{Me} for the temperature interval, where experiment meets difficulties.

Introduction.

Such impurities as Iron, Oxygen, Hydrogen and Silicon considerably spoil Zirconium properties. Various physical methods such, as plasma-arc (PAR), vacuum-arc (VAR) and electron-ray (ERR) remelting have been used now for Zirconium refinement. Method of (ERR) doesn't purify Zirconium from Nitrogen and Carbon and is low effective for Silicon impurities removal. Zirconium purifying by Hydrogen injection into plasma-forming gas are considered in the [1] researches. Impurities removal mechanism usually is explained by its evaporation. Various methods of the high-melting metals refining for the new engineering have been developed successfully and improved during latest ten years. In the process of high purity metal production, such as zirconium, some impurity contents in draft metal exceeds acceptable level determined by technical requirements. Impurities mentioned first of all include Iron, Oxygen, Hydrogen and Silicon [2]. Iron considerably deteriorates Zirconium properties and its removal meets much more difficulties, than other impurities. Various physical methods such as plasma-arc remelting (PAR), vacuum-arc (VAR) [2] and electron ray remelting (ERR) [3, 4] have been used for Zirconium refinement. ERR technology does not refine Zirconium from Nitrogen and Carbon and it is hardly effective for Silicon removal. Researches on Zirconium refinement by means of hydrogen injection into orifice gas are known [1]. Such impurity elements as Fe and H removal from liquid Zirconium in remelting processes have been considered in this work. The basic metal refinement degree from impurity by means of vacuum evaporation in ERR is characterized by refinement factor K_α [5]:

$$K_\alpha = \frac{\gamma p_2^0}{p_1^0} \sqrt{\frac{M_1}{M_2}}, \tag{1}$$

Where γ - activity factor of impurity component: p_1^0 and p_2^0 -saturated vapor pressure of the basic component and impurity; M_1 and M_2 – atomic weight of the basic component and an impurity, correspondingly. Basic component and impurity vapor pressure plays main role in the (1) equation.

Affect of external fields however is known: magnetic field [6] to eutectic Al-Si alloy segregation at 1023K, electric field [7] to the interphase zone Titanium, the crossed electric and magnetic fields [8] to moving of components in Sn-Fe melt.

Molecular Dynamics Calculation.

One of the mathematic simulation methods with computer usage is molecular dynamic (MD), which is more informative and productive than direct experiment in many situations. Sometime, when experimental conditions are very difficult, (high temperature, pressure) it is only method to obtain necessary information. Essence of MD method is motion path calculation of model system particle. The method allow calculate such system property like thermodynamics (energy, pressure), as well as kinetics (diffusion factors, viscosity). Molecular dynamics model consider starting conditions group (array of position and velocities) $\{r_i, v_i, i = 1,…N\}$, which defines state of system in time moment t = 0. Particles number (N) are located in base cell (model cube) with cube side length L in two ways (distribution in the crystal cell nodes and random distribution); initial velocities of the particles are defined depending on initial temperature, which have been defined by researcher. Born- Karman periodic boundary conditions (PGC) are used to avoid boundary effect influence. This treatment considers system of particles as pseudo infinite due to cube under calculation surrounding by its infinite copies number. The particles motion path calculation is carried out basing on specified interaction potential and differential equations of motion. Verlet algorithm with time-step simulation ~ 10 − 15 sec. is used for motion equation discretization. Thermodynamic phase equilibrium is divided by macro and micro steps to calculate mean values and dispersions. This phase micro-characteristics (particles coordinates and velocities of the system) are used for macroscopic properties: potential, kinetic and total energies, temperature, pressure, thermal capacity, kinetics factors of transfer.

Molecular dynamic method had been used in the present work for Iron and Zirconium diffusion factors dependence on electric field and Hydrogen presence in the Zirconium melt analysis. Molecular dynamics (MD) method modeling had been carried out using micro canonical (NVT) ensemble. Model system used in MD method for research of iron and hydrogen ions behavior in the Zr-Fe-H melt at T=2273K temperature and an electric field, has been presented by 516 particles of zirconium, 60 particles of iron and 1 particle of hydrogen in a cubic cell with the cube edge length a=2.44195 nanometer. The model system, used in MD method for Hydrogen behavior in Nb-H melt at T=3200K, was presented by 1000 Niobium particles and 10 Hydrogen particles in cubic cell. Periodic boundary conditions have been used. Movement equations integration was carried out by $1.1 \cdot 10^{-15}$ sec. time step using Verlet method [9]. The particles of system had been placed randomly in basic MD cell before modeling. Interpartial potentials and potentials factors numerical values have been used from works [10, 11]. Interaction in the MD-models had been defined as resulting force of pair interaction potentials in the pair models approximation. Temperature of system had been found from the total kinetic energy of system. Diffusion factors D of zirconium, iron and hydrogen impurities have been calculated as model particles mean square displacement $\langle \Delta R^2(t) \rangle$ for the great number of steps.

Short Order. Short order of the disorder systems is described by radial distributions function of atoms g(r) (RDF), which determines any atom location probability on distance r from fixed atom [12]. The results of impurity migration calculations in liquid zirconium are compared to the experimental data [1-4]. Partial radial distribution functions $g_{ij}(r)$ of zirconium-iron melt are presented in fig.1. Most probable distance between atoms in the first coordination sphere appears close to the sum of atomic
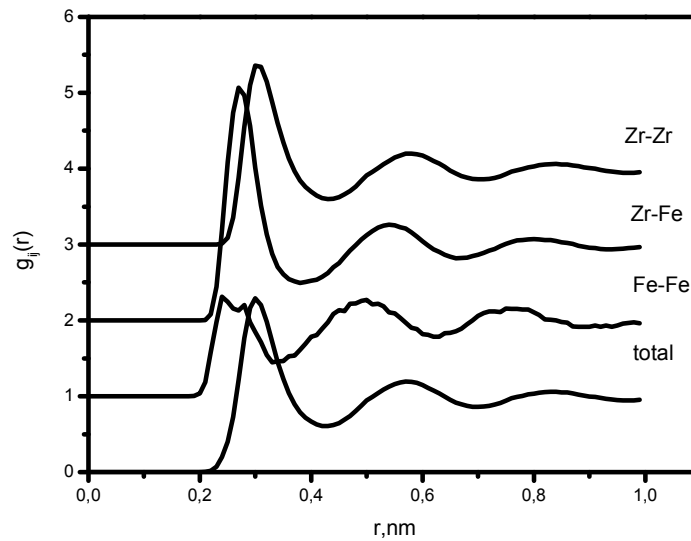
Fig.1. Partial radial distribution functions g_{ij} (r) of Zr-Fe melt at 2273K, obtained in the MD model.

radii of iron and zirconium (r_{Zr-Fe}=0.29nm, r_{Fe}=0.130nm, r_{Zr}=0.162nm). Comparison of these results with our data on computer calculation of Ta-Fe melt [13,14] gives enough close agreement to the distribution functions of big size atoms namely Ta-Ta (0.29 nm, r_{Ta}=0.145nm) and Zr-Zr (0.324nm, r_{Zr}=0.162nm).

Diffusion factors. Iron and zirconium diffusion factors in zirconium melt at 2273K temperature at the presence and without electric field and hydrogen have been calculated by molecular dynamics method (fig. 2 and 3). Diffusion factor of iron (D_{Fe}) in zirconium melt with hydrogen linearly increases with electric field intensity (E) and iron concentration (C_{Fe}). The hydrogen diffusion factor negligibly decreases from $2.16 \cdot 10^{-4}$ $cm^2 \cdot s^{-1}$ up to $1.94 \cdot 10^{-4}$ $cm^2 \cdot s^{-1}$ at E increase from 900 up to 1020V/m. Hydrogen introduction in system at $C_{Fe} \approx 0.1\%$ decreases D_{Fe} value from $7.86 \cdot 10^{-5}$ to $6.36 \cdot 10^{-5} cm^2 s^{-1}$, and electric field imposing of 1020 V/m intensity decreases D_{Fe} to $5.22 \cdot 10^{-5} cm^2 s^{-1}$ (fig. 3). The results of D_{Fe} variation calculation by MD method linked with E value been compared to speed constant of Fe ions from Zr evaporation, calculated by the equation [15, 5]

$$k = v \cdot C_{Fe} \exp\left[-\frac{\lambda + I - W - (q^3 \cdot E)^{1/2}}{RT} \right],$$ (2)

Where v – fluctuation frequency of ion – ($10^{13} \cdot c^{-1}$), C_{Fe} - impurity concentration, λ – evaporation heat of Fe, I – the first ionization potential (B/$\overset{0}{A}$), E - electric field intensity, W – electron exit work, q – charge of ion. Values λ, I, W, R are presented in electron - volt, E - volt per angstrom. The Diffusion factor D is in direct dependence on speed (k) and time (t) evaporations of the basic metal [16].

Dependences of log k and log D on E (fig. 4) are relatively close. Therefore it is possible to speak about approximately identical form of k and D curves. It seemingly, allows consider diffusion of Fe as limiting stage of Fe removal from the Zr – melt. Problem of hydrogen diffusion as light intrusion-type hydrogen presence at 2273K temperature.

impurity in the metals with different lattice type is important in the researches of high-temperature refinement of metals. Some metals (Ti, Zr, Nb, Ta, Pd, etc.) are characterized by high Hydrogen solubility limit and form hydrides. Metals of VI, VII groups, noble metals, Fe, Zr, Nb, Ta, Pd, etc. have negligible solubility limit and positive dissolving enthalpy [17]. Hydrogen is dissolved in metals during melting, casting and other technology processes. This phenomenon is one of the reasons, which lead to defects occurrence and metal properties deterioration. Incoherent diffusion is dominant at high temperature and impurities negligibly affect to it [18].
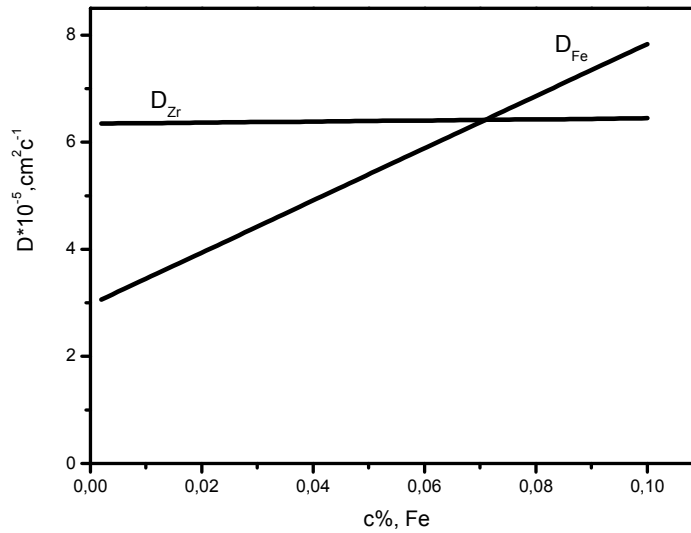

Fig. 2. Dependence of D_{Fe} and D_{Zr} on iron concentration (MD calculation).
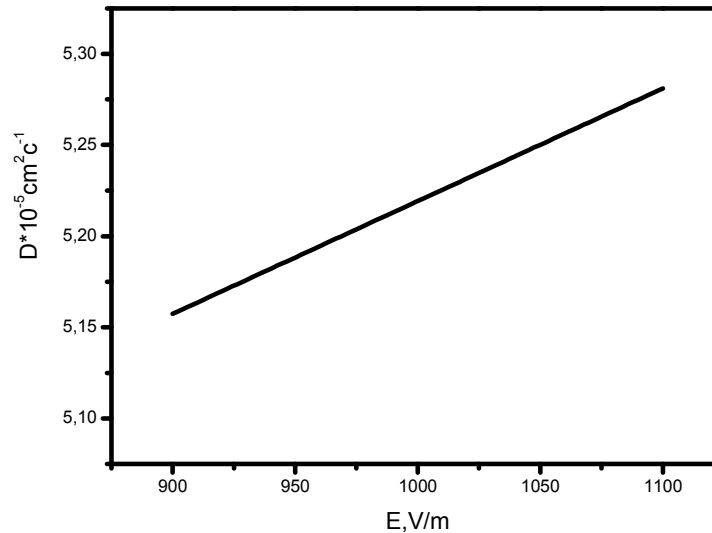

Fig.3. Dependence of iron diffusion factor (C_{Fe} =0.1mas. %) on electric field intensity (E) and hydrogen presence at 2273K temperature.

Many experimental and theoretic researches on Hydrogen diffusion in the pure metals D^{Me}_H up to 700K (Me=Ta, Zr, Nb) are known. The difficulties of reliable D_H data obtaining increase at the temperatures close to melting. Meanwhile values of D_H at high temperatures play significant role in

various technical applications. As an example, recent years researches of plasma arc melting at various Hydrogen medium pressures of the high melting metals are carried out [19]. Interesting application sphere is membrane producing for Hydrogen refinement [20].
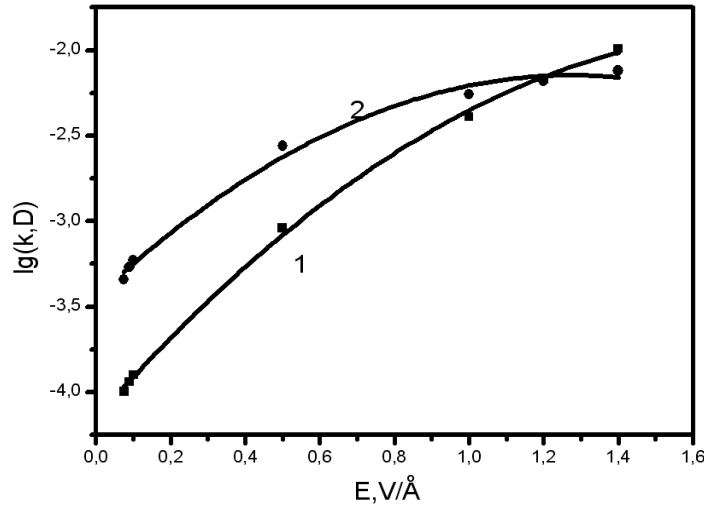

Fig.4. Dependence of lgD (curve 1) and lgk (curve 2) on electric field intensity.

Thereupon systematization of the diffusion data on Hydrogen in the certain high-melting metals at temperatures close to melting (T_m) and in molten state is necessary. There are data on density (ρ) and diffusion factors (D_H) for some metals in solid and liquid state. This data are presented in the table 1 and by fig. 5. This data analysis allows consider D_H^{Me} as linear function of density characterized by equation (3) with ±0.84 accuracy:

$$\lg D^{Me}_H = 0.1376\rho - 3.7577 \qquad (3)$$

Using (3) equation we calculated D^{Me}_H for Zr, Nb and Ta melts depending on its densities. Calculation of D^{Me}_H (Me=Ta, Zr, Nb) in molten state can be carried out by Arrhenius equation extrapolation to T_m, considered in [21-23] for temperature interval 700 – 1000K. Direct extrapolation up to T_m and higher, however, gives inadequate result. Therefore Gorsky effect was taken into account using proportional relation $\Delta \lg D^{Me}_H / \Delta T^{-1}\ 10^4$ to the same relation above 1000K according to [24]. Thus
we managed to obtained D_H change value at Zr, Nb and Ta melting.

Table 1. Hydrogen diffusion factors for various metals.

Metal	Ni[25]	Zn[26]	Fe[25]	Cu[25]	Ag[25]	Zr [MD,calc.]	Nb [MD. calc]	Ta[27]
T, K	1811	1811	1811	1811	1811	2273	3200	3400
ρ,g/cm^3	7.75	6.8	6.98	7.62	8.82	6.64	8.0	15
D_H, cm^2/s	$7.08\cdot10^{-4}$	$2\cdot10^{-3}$	$1.4\cdot10^{-3}$	$6.03\cdot10^{-3}$	$3.09\cdot10^{-3}$	$5.01\cdot10^{-4}$	$1.1\cdot10^{-3}$	$2.93\cdot10^{-2}$
LgD_H^{Me}	-3.15	-2.7	-2.85	-2.22	-2.51	-3.3	-2.97	-1.53

We extrapolated Hydrogen diffusion factors data of Zr[21], Nb[22] and Ta[23] in 700 – 1000K interval to the melting temperatures region. Calculation of D_H in Ta [27], Zr and Nb [this research] have been carried out by molecular dynamic method. Our results obtained accounting Gorsky effect are compared with MD calculation for molten state and D_H change value at melting temperatures of this metals was obtained.

Right extrapolation from 700 up to 2273K (without Gorsky effect accounting) of known D_H values for Zr leads to very close values to those of MD calculation method for molten state. Similar extrapolation up to 3200K for Nb gives overestimated data, and underestimated value for Ta (fig.6). According to Gorsky effect for Deuterium [24] at 1000K break of line is observed, which leads to decreasing of D^{Me}_H values at T>1000K. Basing on this data and applying it to Hydrogen we obtain decreased values of D^{Me}_H (Me=Ta, Zr, Nb) at melting temperature (T_m). Change of D^{Me}_H values at T_m in all cases can be obtained. This change value for Zr is one order, about 1/3 order for Nb and approximately two orders for Ta. It should be noted, that density changes are also observed at T_m for all three metals. Thus our calculation data of D^{Me}_H in molten state for considered three metals Ta, Zr, Nb with assumed terms are in good agreement with recent conception about temperature permutation of D_H in Zr, Nb and Ta up to molten state.

Correctness of the Gorsky effect accounting for solid Nb is confirmed by the slope of lgD_H^{Nb} – 1/T dependence, obtained by the MD method [28, 29]. This right line for Niobium is close to the dependence, calculated from Gorsky deduction. Our carried out analysis allows to define the direction
and position of lgD_H^{Me} right line for three researched metals in the temperature region, where necessary experimental data are absent.
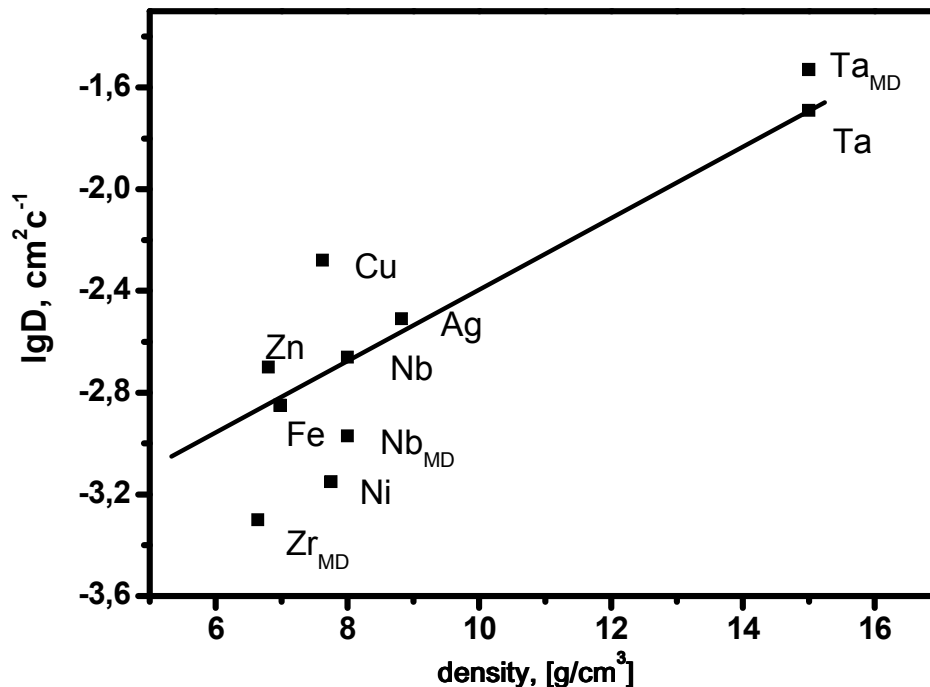

Fig.5. Dependence of LgD on metals density by experimental data.
(Calculation by equation (1) for Zr, Nb, Ta; calculation by MD method for Zr_{MD}, Nb_{MD}, Ta_{MD})
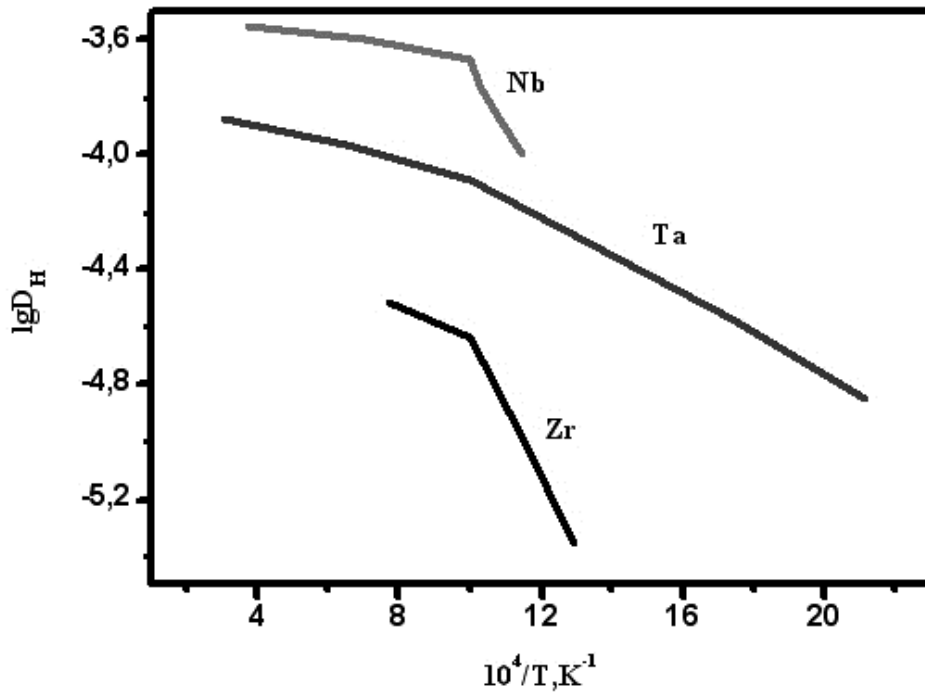
Fig.6. Dependence of LgD_H on inverse temperature for Zr, Nb and Ta.

Incoherent diffusion became dominating at high temperature and impurities smaller affect to diffusion process [30]. We had compared diffusion factors of hydrogen at 3400K temperature in Ta [13] and in Zr at 2273K. They appeared to be equal $1.7 \cdot 10^{-5}$ and $5.01 \cdot 10^{-4} cm^2 \cdot s^{-1}$ respectively. Authors [30], explain such divergence due to diffusion activation energy dependence of hydrogen (E_a) on atomic weight of metal, its Debye frequency, elasticity modules and volume change in the case of hydrogen addition. Calculated E_a values for various metals [31] conform quantitatively to the experimental data. Temperature dependence of D_H at high temperature is described by the theory [31]. It is shown [32], that D_H in zirconium without electric field at 2273K temperature is $3.862 \cdot 10^{-4} cm^2 \cdot s^{-1}$, which slightly differs from $D_H = 5.01 \cdot 10^{-4} cm^2 \cdot s^{-1}$ value calculated in the present work.

Diffusion layer. On the basis of experimental dependence C_{Fe} on time [4] using D_{Fe}, calculated by MD method, we have estimated diffusion layer thickness *(x)* by the equation [31]

$$C_{(x,t)} = C_0 erfc\left(\frac{x}{2 \cdot \sqrt{D_{Fe} \cdot t}}\right), \qquad (4)$$

Where C_0 and $C_{(x, t)}$ – impurity contents in initial and refined zirconium [4], t – time of refining. Obtained *x* – value is $7 \cdot 10^{-2}$ cm. By the order of value it's close to the data [33] $1.6 – 1.8 \cdot 10^{-2}$ cm, related to silicon borating. We obtained the diffusion zone thickness of zirconium shell interaction with the molten uranium is $0.2 \cdot 10^{-2}$ cm[34].

We carried out calculation of iron removal speed from zirconium (G) by the iron concentration decreasing during corresponding remelting time intervals: beginning (within 0 h 30min.), middle (within 75 h 105min.) and the end (within 150 h 180min.) in the PAR process with 50% hydrogen in the residual argon using experimental data [4] for 9.5 Pa. The average residual iron content at 15, 90 and 165 minutes was 0.46, 0.01 and $2.2 \cdot 10^{-4}$ mass% respectively. These calculations are compared to speed of iron evaporation from zirconium melt by Langmuir equation:

$$L = 0.0583\gamma C_{Fe} cp \sqrt{\frac{M}{T}} \,, \tag{5}$$

Equation parameters are: γ – iron activity factor in zirconium 0.052 from [2], C_{Fe} – Fe concentration in Zr, p – iron vapor pressure at 2273K, M – iron atomic weight, T – Kelvin's temperature. Remelting temperatures in [4] are presented within the 2350 - 2450K limits. Calculation of L by these temperatures shows, that in both cases L <G. With the temperature increase G/L decreases. Obtained $G/L \approx 1.15$ at C_{Fe}=0.46 and T = 2450K can specify that about 15 % of iron have been removed due to electromagnetic forces affect but the evaporation.

Summary

Process of the molten zirconium refinement has been analyzed by molecular dynamics method. The analysis allowed estimating limit stage of process, electric field intensity and iron impurity affect to its diffusion factor D_{Fe} in liquid zirconium. Calculation of Iron evaporation speed from Zr melt considering initial iron concentration is compared to real iron removal from zirconium in ERR, PAR with hydrogen and VAR remelting processes. Speed of impurity removal is approximately proportional to iron diffusion factor up to the middle of remelting process. Further Fe removal probably depends on hydrogen presence in plasma-forming gas and electric field intensity.

Based on Hydrogen diffusion factors in molten Ni, Zn, Fe, Cu, Ag dependence of D_H^{Me} on metals density at 1811K temperature is obtained. Proper equation is used for D_H^{Me} (Me=Zr, Nb, Ta) values calculation from density of Zr, Nb and Ta at 200 – 300K above its melting temperatures. Comparison of the D_H^{Me} (Me=Zr, Nb, Ta) values, calculated by two different ways, revealed satisfactory convergence.

Acknowledgment

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