THERMAL EFFECT AND STRESS SIMULATION IN ZIRCONIUM AFTER PULSED PLASMA IMPACT

V.I. Shymanski, Zhang Zeyu
Belarusian State University,
4 Nezavisimosti Ave., 220030 Minsk, Belarus, shymanskiv@mail.ru

In the work the results of simulation of temperature distribution in zirconium after pulsed plasma treatment are presented. The plasma treatment is widely used for materials modification that takes place in melting mode. To choose the plasma parameters for melting of the top layer the simulation was provided. In the proposed model the phase transformation in zirconium connected to transformation from solid phase to liquid was taken into account as a special function of heat capacity. The obtained results showed the absorbed energy density should be higher than 12 J/cm^2 for starting melt of the surface. After plasma pulse, the top layer begins to solidify with high cooling rate and speed of crystallization front motion. Besides, the high level of temperature gradient provides mechanical stress inside which reach 1.0 GPa.

Keywords: zirconium; plasma treatment; heating simulation; stress simulation; cooling rate.

Introduction

Low neutron absorption cross-section, attractive mechanical properties and good corrosion resistance make zirconium (Zr)-based alloys the best possible cladding material in modern thermal nuclear reactor. These materials displayed a very good combination of properties such as low neutron sorption, stress-corrosion cracking resistance, creep behavior, and reduced corrosion.

It is well known that there is water corrosion, neutron irradiation and relatively small amounts of hydrogen as solid solution, which in turn leads to degradation of mechanical properties. The presence of high temperature, high pressure and mechanical load further more induces degradation of mechanical properties of zirconium alloys.

Therefore, it is urgent for the nuclear industry to explore an appropriate method to optimize the surface corrosion resistance performance to enhance the accident tolerance.

With in the process of high energy pulsed plasma beam, a high energy is instantaneously deposited to the surface layer, and induces extremely fast heating, and melting then rapid cooling and solidification. In this case, significant modifications within the irradiated layer such as phase transformation, grain refinement, surface homogenization and element redistribution etc. can be easily obtained. Simultaneously, abundant structure defects can be also generated.

Given this, in present work, a detailed characterization work was performed to the energy transmission, phase transformation and stress distribution in the surface layer of zirconium after plasma treatment by simulation. It will present a guiding role in the practice of specific practical operations and modifications and contribute to the analysis of the mechanism.

Experimental

Based on Comsol 5.6 software, the material considered is Zr_7O_2 plate cut into small sized (0.1×0.1×1 mm). Pulsed plasma beam with absorbed energy densities 10 – 50 J/cm^2 and pulse duration 100 μs applied to 0.1×0.1 mm side of the Zr plate. To take into account the latent heat amount during phase transformation when solid state transforms into liquid state the heat capacity of Zr was set by the temperature-dependent function (the temperature ranges are provided °C scale):

$$c = \begin{cases} 240 + 0.127T, & 273 < T < 2126 \\ 3689 \cdot \exp\left[-\dfrac{(T-2128)^2}{5.8} \right], & 2126 < T < 2130 \\ 254 + 0.051T, & 2130 < T < 7000 \end{cases}$$

The middle part of the heat capacity function c uses gaussian function to simulate the melting heat of Zr and to tolerate the accuracy of the software.

The heat transfer equation considered in the simulation is

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T \right) + Q \, ,$$

where ρ is the density, c is the heat capacity, T is the temperature, t is the time, k is thermal conductivity, Q is the heat source.

After cooling of the surface layer of the materials, high level of mechanical stress arises. To estimate the stress, the following equation was solved:

$$\nabla \cdot S + F_v = 0 \, ,$$

where S is the stress, F_v is the deformation gradient tensor. As the mean reason of the stress appearance is the linear expansion, the deformation ε_{th} was calculated as follows:

$$\varepsilon_{th} = \alpha \left(T - T_{ref} \right) ,$$

where ε_{th} is the thermal strain, α is the coefficient of thermal expansion.

Based on the above conditions, finite element simulation analysis is performed.

Results

The plasma action on the surface of zirconium metal was calculated by simulation for different energies (10 – 30 J/cm^2) within 0.1 ms. The temperature versus time curves of the zirconium metal surface and the temperature versus time curves inside the zirconium metal at the time just after the plasma treatment were calculated.

As we can see by Figure 1, the surface of zirconium metal can reach its melting point only when the energy of the plasma is greater than 12 J/cm^2. Due to the extremely short action time of the plasma, the plasma action can bring the surface layer of zirconium

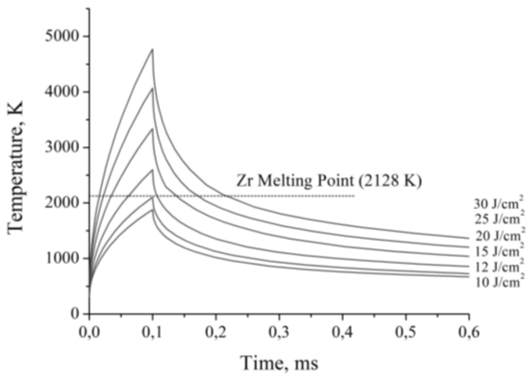

Fig. 1. Zr surface layer temperature with time under different plasma energy impact

metal to a high temperature. Moreover, the temperature of the surface layer drops very quickly. The heat energy is quickly transferred by the metal to a larger volume and is stabilized at a lower (below melting point) temperature.

Figure 2 shows the temperature distribution of the zirconium metal surface at a depth of 50 μm just after the plasma treatment. From Figure 1, the highest temperature of the metal surface is just after the plasma treatment, so the temperature distribution is more representative.

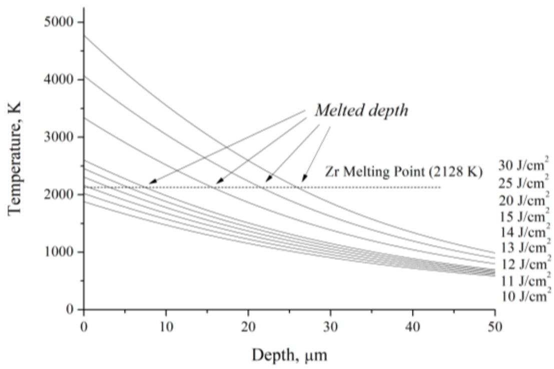

Fig. 2. Temperature with depth after heating under different plasma energy

By looking at Figure 2, the depth of the melting layer on the metal surface becomes deeper with increasing energy very significantly. The depth increases more linearly with a certain attenuation, which may be due to the higher the temperature, the faster the dissipation of energy. At 25 J/cm^2, the surface melting depth can already reach about 21 μm, and this thickness can already form a thicker modified layer on the metal surface.

With the data in Figure 3, the rate of cooling can be calculated for a very small period of time (50 μs) after the plasma treatment is completed. It can be seen from the figure that the rate rises linearly with the growth of the plasma energy. It can be seen that the higher the temperature the faster the energy transfer, which can be somewhat linear in the range of plasma heating. And this can be used to consider its surface grain growth and stress distribution.

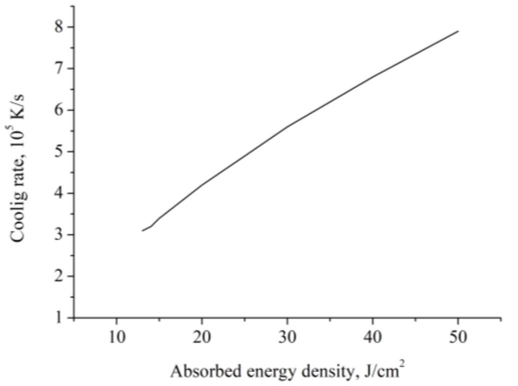

Fig. 3. Cooling rate with different plasma energy

Figure 4 shows the images of the stress distribution with depth at different times after plasma treatment for a metal surface layer of 100 μm depth. Since the previous data we can know that the temperature change is more obvious in the surface layer 50 μm depth, so we focus on the stress distribution in the first 100 μm.

From the figure we can see that the stresses inside the material at the end of the plasma treatment are extremely high, up to the order of 1.0 GPa, due to the thermal expansion of the material, and propagate to the right during the heat transfer. Due to the presence of melting of the metal into liquid state, there is a clear inflection point in this

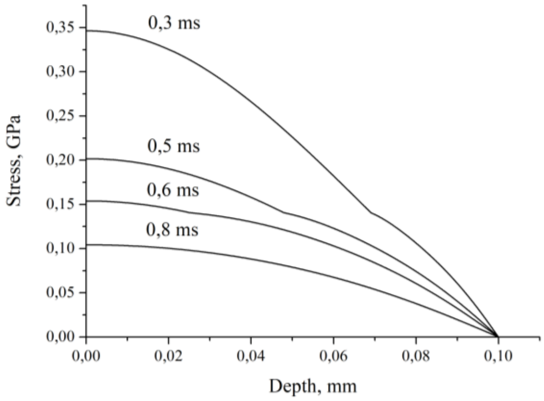

Fig. 4. Stress distribution with depth at different time with 20J

image, while to the left of the inflection point the metal is in liquid phase and should not be discussed in the stress problem. It is observed from the figure that the stress can reach 0.1 GPa order of magnitude in 1 ms of time, and the stress changes rapidly with temperature. And the decay of stress is not uniform with time, from a faster decay rapidly weakening to a slower decay level, where the time distribution of heat transfer can be referred to.

Conclusions

The present work showed the possibility of zirconium melting by the pulsed impact with plasma stream at absorbed energy density more than 12 J/cm^2 at pule duration 0.1 ms. The simulation procedure took into account the phase transformation by means of heat capacity change. The results showed the high cooling rate of the zirconium melt which reaches $8 \cdot 10^5$ K/s after plasma pulse. Such big value of cooling provides nonuniform thermal expansion of the top layer and stress arising.