In-situ observation of dislocation and analysis of residual stresses by FEM/DDM modeling in water cavitation peening of pure titanium

DY Ju1,2 and B Han2
1 Department of Material Science and Engineering, Saitama Institute of Technology, Japan
2 Department of Mechanical Engineering, University of Science and Technology Liaoning, Qianshan load 184, Anshan, China
E-mail: dyju@sit.ac.jp

Abstract. In this paper, in order to approach this problem, specimens of pure titanium were treated with WCP, and the subsequent changes in microstructure, residual stress, and surface morphologies were investigated as a function of WCP duration. The influence of water cavitation peening (WCP) treatment on the microstructure of pure titanium was investigated. A novel combined finite element and dislocation density method (FEM/DDM), proposed for predicting macro and micro residual stresses induced on the material subsurface treated with water cavitation peening, is also presented. A bilinear elastic-plastic finite element method was conducted to predict macro-residual stresses and a dislocation density method was conducted to predict micro-residual stresses. These approaches made possible the prediction of the magnitude and depth of residual stress fields in pure titanium. The effect of applied impact pressures on the residual stresses was also presented. The results of the FEM/DDM modeling were in good agreement with those of the experimental measurements.

1. Introduction
Cavitation impact has historically attracted attention due to its costly damage to hydraulic mechanical parts, such as hydrofoil surfaces, turbopump impellers, pumps, and valves. As such, many researchers [1-5] have traditionally focused their investigations into the damage mechanism of cavitation.
More recently, cavitation impact has been successfully developed as a means to improve the fatigue performance of mechanical components by introducing residual stress into the superficial layer of metallic components, in a manner similar to the more conventional process of shot peening. Ju and Qin et al. [16] designed a new ventilation nozzle, through which suitable air can be aerated into the extra high-velocity flow in the nozzle throat, thereby forming a tremendous pressure gradient between the upstream and downstream flows. This specific method is referred to as water cavitation peening (WCP) [6, 7]. Sahaya Grinspan and Gnanamoorthy successfully employed another cavitation process by injecting a high-speed oil jet into an oil-filled tank. This method, referred to as oil jet peening (OJP), effectively reduces the erosion of mechanical components [8-10]. Several recent investigations have revealed that WCP improves fatigue performance by introducing compressive residual stresses in the surface of metallic components [7- 9, 11, 12]. The method has also been demonstrated to induce high uniform compressive residual stresses in gear tooth surfaces, since complicated and narrow surfaces can be more easily peened [16]. Compared with conventional shot peening, WCP can obtain the smoother surfaces. The distributions of impact pressure are isotropic, therefore, process capability of WCP is uniform at different incidence angle [16]; however, it is unknown if WCP can induce changes in the microstructures within the strengthened layers of metallic components, as shot peening does [18- 21].
Residual stresses in materials are often the result of metallurgical processes, such as casting,
forging, welding, and quenching. Residual stresses from metallurgical processes usually depend on changes in thermal sources and volume accompanying the phase transformation. Generally, two types of residual stresses should be considered, that is, macro-residual stresses and micro-residual stresses [23]. Macro-residual stresses depend on the plastic deformation of solid materials due to rapid non-uniform cooling, while micro-residual stresses are caused by strain and deformation due to phase transformation and changes in microstructure. We also know that distortions due to thermal and elastic-plastic deformation and strain, as well changes in phase transformation and texture in manufactured materials, are important regardless of the type of residual stresses. Unfortunately, since the post-WCP distortion process is minimal, it is not sufficiently clear why the WCP process creates such large compressive residual stresses, similar to traditional peenings. Therefore, it is important to clarify the cause of residual stress generation through basic material properties research.

In order to approach this problem, specimens of pure titanium were treated with WCP, and the subsequent changes in microstructure, residual stress, and surface morphologies were investigated as a function of WCP duration. The influence of water cavitation peening (WCP) treatment on the microstructure of pure titanium was investigated. The microstructural evolution in the near-surface of pure titanium as a function of WCP time was characterized by X-ray diffraction (XRD), optical microscopy (OM), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). After WCP treatment, changes in the microstructure, as well as residual stress and surface morphologies as functions of WCP time, were recorded using a novel experimental design involving an in-situ observation function. The obtained results indicate that twinning plays an important role in the plastic deformation and residual stresses of hexagonal close-packed (HCP) structured metal materials, and therein, that the deformation twinning and twinning interaction were induced by WCP in the strengthening layer. A stable compressive residual stress layer was found in the near-surface of the investigated pure titanium.

In this paper, a novel combined finite element and dislocation density method (FEM/DDM), proposed for predicting macro and micro residual stresses induced on the material subsurface treated with water cavitation peening, is also presented. A bilinear elastic-plastic finite element method was conducted to predict macro-residual stresses and a dislocation density method was conducted to predict micro-residual stresses. These approaches made possible the prediction of the magnitude and depth of residual stress fields in pure titanium. The effect of applied impact pressures on the residual stresses was also presented. The results of the FEM/DDM modeling were in good agreement with those of the experimental measurements.

2. Experimental procedures
2.1. Test specimen and WCP conditions
Fig. 1 depicts a schematic of the test specimen and clamp. The test specimens consisted of pure titanium in as-annealed process state. The size of each test specimen was 4 mm × 6mm × 32 mm. The special clamp depicted in Fig. 2 was used to ideally combine the specimens (A) and (B) into one part.

The key process conditions of WCP include aeration flux, standoff distances (SOD), and WCP duration. All of these attributes significantly impact the degree of enhancement of the process, and therein, it is necessary to determine ideal process conditions prior to treating the test specimens. According to recent observations[15] regarding impact pressure distribution measurements, an aeration flux of 0.4 L/min and a SOD of 85 mm were demonstrated to induce a tremendous impact pressure. As shown in Fig. 2, the specimens were treated by WCP in the bottom center of the test water tank. WCP durations of 15 min, 30 min, 45 min, and 60 min were investigated in this study.
2.2. OM observation of microstructures
The specimens A and B were first ground and polished, and the surfaces of the microstructure observation points were eroded with a solution of 10% HF + 5% HNO₃ + 85% H₂O. The microstructure photos showing the different optimal points were recorded by OM. As depicted in Figs. 1 and 2, the same two specimens were joined by the special clamp in the WCP process. Finally, the microstructures at the same points were again recorded by OM after the WCP treatment. In the preceding method, microstructural changes in the superficial layer were recorded at each step for each WCP duration.

2.3. TEM observation of microstructures
The TEM (JEOL2100) was used to examine specimen microstructures at a depth of 30 to 40 μm from the surface in order to further investigate any microstructural changes due to the WCP treatment. In order to obtain a clear image of the microstructure, samples were observed using SEM after etching in a solution containing 10%HF + 5%HNO₃ +85%H₂O. A Twin-Jet Electropolisher (FISCHIONE-140 Digital Power Control) and a solution of 5% HClO₄ + 95% CH₃OH was used to etch the specimens to an optimal thickness for TEM analysis.

2.4. Residual stress measurement
The surface residual stress and depth distribution of residual stress in the near-surface layer were measured by X-ray diffraction stress analysis using the conventional sin²Ψ method. A special optical system jointly extracted precise information concerning the residual stresses in areas as small as 0.15 mm in diameter. In this study, a side inclination method was also used for stress measurement. The X-ray tube (Co-Kα type) was operated at 30 kV and 10 mA, with a slit diameter of 2 mm. The shift of the α-Ti (114) diffraction profile was detected at angles Φ = 10°, 20°, 30°, 40°, and 45°. The diffractive angle 2θ₀ was 154.4°. The stress constant of the X-ray diffraction analysis was −180 MPa/°. Moreover, Vickers hardness was measured on the peened surface (peened for 45 min) and unpeened specimens with a load of 9.8 N. In order to investigate the depth distribution of the residual stress, the near-surface layer of the test point was removed by step-by-step electrolytical polishing using a Proto Electrolytic Polisher-Model 8818 (Proto Manufacturing Ltd.). The depth of the electrolytic polishing was approximately 10 to 25 μm at each step, and was adjustable via the voltage control, timer control, and flow rate of the electrolyte control. The depth distribution of the residual stress was obtained by measuring the residual stress at each step.

3. Analysis Model by FEM/DDM
Considering not only macro-plastic strain but also micro-plastic strain, the total residual stress $\sigma_{\text{residual}}$ induced by WCP is given by
\[ \sigma_{\text{residual}} = \sigma_{FEM} + \sigma_{DDM} \]  
(1)

where, \( \sigma_{FEM} \) is the resolved residual stress induced by macro-plastic deformation, which can be obtained from the finite element method; and \( \sigma_{DDM} \) is the resolved residual stress induced by macro-plastic deformation, which can be obtained from the dislocation density method. Under uniaxial strain conditions, the highest elastic stress level in the impact wave propagation is defined as the Hugoniot Elastic Limit (HEL). According to Hook's law \([27]\), the surface plastic strain \( \varepsilon_p \) can be expressed as

\[ \varepsilon_p = \frac{-2\text{HEL}}{3\lambda + 2\mu} \left( \frac{P}{\text{HEL}} - 1 \right) \]  
(2)

where, \( P \) is the impact pressure and a function of pressure pulse duration, \( \lambda \) is Lame's constants, and \( \mu \) is Lame's constants. The residual stress \( \sigma_{FEM} \) induced by WCP can be written as

\[ \sigma_{FEM} = \sigma_0 - \left[ \frac{\mu \varepsilon_p (1 + \nu)}{(1 - \nu)} + \sigma_0 \right] \left[ 1 - \frac{4L_p (1 + \nu)}{\pi r_p} \right] \]  
(3)

where, \( r_p \) is the radius of circular impact zone on the target, \( \sigma_0 \) is initial residual stress, and \( L_p \) is the depth of plastic affection.

\[ \sigma_{DDM} = -A\mu b \sqrt{N_m} + \sigma_0 \]  
(4)

where, \( \sigma_{DDM} \) is the residual stress induced by dislocations; \( A \) is the constant caused by unknown sources; \( \mu \) is the shear modulus; \( N_m \) is the density of mobile dislocation; \( b \) is the magnitude of Burgers vector, and \( \sigma_0 \) is the original stress. According to Eq. 2 and Eq. 1, the total residual stress \( \sigma_{\text{residual}} \) can be written as

\[ \sigma_{\text{residual}} = \left[ \frac{\mu \varepsilon_p (1 + \nu)}{(1 - \nu)} + \sigma_0 \right] \left[ 1 - \frac{4L_p (1 + \nu)}{\pi r_p} \right] - A\mu b \sqrt{N_m} + \sigma_0 \]  
(5)

Based on Eq. 1, the total residual stress \( \sigma_{\text{residual}} \) induced by WCP can be obtained by the combined finite element method and dislocation density method (FEM/DDM) approach.

4. Results and discussion

4.1. Microstructures

The microstructural changes of the superficial layers as a function of WCP duration, at the same observation points, are shown in Fig. 3. Figure 3 (a) depicts typical equiaxial \( \alpha \) grains of annealed pure titanium, with grain sizes in the range of 20 to 100 \( \mu \)m. From Fig. 3 (b-d), the microstructural evolution of the titanium specimens at WCP durations of 15 min, 30 min and 45 min can be clearly observed. The deformation twinning induced by WCP at a depth of 30 to 40 \( \mu \)m from the surface can be observed via the OM micrographs in Fig. 4 (a,b). The density and quantity of deformation twinning increase gradually with increasing WCP duration, and decrease gradually with increasing layer depth from the treated surface. The density and quantity of deformation twinning no longer significantly increase when the WCP time exceeds 45 min and when the depth of deformation twinning reaches approximately 150 \( \mu \)m. The trend in microstructural change is similar to that of the compressive residual stress. At the same time, the integrity of the treated surface is maintained, proving that WCP can produce a smoother surface with minimal structure losses.

The TEM microstructures at a depth of 30 to 40 \( \mu \)m are depicted in Fig. 5. The interaction of deformation twinning in two different directions, as well as the high density dislocations among the bands of twinning, can be seen in Fig. 5 (a). Three types of twinning systems cross at the same point, as shown in Fig. 5 (b).
4.2. Residual stress
The typical residual stress distributions in the superficial layers, as functions of WCP duration, are depicted in Fig. 6. From Figure 6, it can be observed that the maxima of the compressive residual stresses due to WCP are at the surfaces of the specimens for all of the investigated WCP treatment durations. This observation result differs from that of shot-peened. The maximum residual stress is usually observed below the surface during the shot-peening process. The distributions of compressive residual stresses depend on material characteristics and peening conditions. Furthermore, the load mode of WCP is an impact wave pressure due to cavitation collapse. The obvious macro-non-uniform plastic deformation is not induced by WCP, as compared to the deformation one would observe in other traditional methods. Crystalline defects, such as vacancies, interstitials, dislocations, and twinning, are the primary causes of compressive residual stress distributions during WCP process. The maximum of compressive residual stress observed was –620 MPa at a WCP duration of 60 min. As the depth from the surface was increased to 150 µm, the compressive residual stress was observed to gradually decrease. In comparison to residual stress distributions of WCP-treated specimens, those of original specimens essentially show zero residual stress throughout the entire near-surface. Since the compressive residual stress was observed to slowly increase after 45 minutes, this can be considered as the saturation time of compressive residual stress. This result indicates that the compressive residual stress can be induced in the near-surface of the specimen through WCP. Vickers hardness measurements were conducted on the peened (45 min) and unpeened specimen surfaces to evaluate their respective hardnesses. Table 2 depicts the changes in surface hardness of the peened and unpeened specimens, and therein, the average hardness of the peened specimens was about 17 HV higher than that of the unpeened specimens, indicating strengthening due to WCP.

4.3. Analysis results of residual stress by FEM/DDM model
According to the predicting method proposed in this paper, the residual stress distributions were predicted after 45 min with the different applied impact pressures. Figure 7 shows the predicted results of residual stress after 45 min with the different applied impact pressures. The black line indicates the predicted results based on the EFM model, while the red line represents the prediction results based on the DDM model. The green line shows the total residual stresses based on the FEM/DDM model. In Fig. 7, the predicted results with different applied impact pressures after 45 min and the experimental results measured by XRD method are compared. The predicted results considering the macro-residual stress and the micro-residual stress with applied impact pressure around 800 MPa are in good agreement with the experimental results by XRD method. These results indicate that the new model could potentially be a useful tool in predicting the residual stresses and investigating the effect of processing materials parameters on the distribution of residual stress.

4.4 Strengthening modeling and mechanism of WCP
Fig. 8 illustrates the proposed mechanism of WCP, and depicts the strengthening model of the surface microstructure for a pure titanium plate during the WCP process. The modeling is based on the residual stress concentration generated by a pile-up caused by a dislocation activation of the impact source [21-26], such as that shown in Fig. 8. The amount of dislocation-induced pile-up is determined by the distance L between the dislocation lines created by the source and barrier, and the applied stress. The local stress in front of the barrier is equal to the product of the initial residual stress and the number of piled-up dislocations. The unique twinning that is created will strongly depend on micro-residual stresses and dislocation-induced pile-up. The initiation and propagation of the twinning in a neighboring grain are also shown in Fig. 8. The crystal structure of pure titanium is a typical HCP structure at room temperature. The basal planes (0001) are the close-packed planes, and there are three close-packed directions <1120>; hence, in HCP, there are three slip
systems. This low number of slip systems means it is difficult to plastically deform an HCP metal. It can be shown that five slip systems must operate in each grain of a polycrystal if it is to deform in a manner compatible with the deformations of its neighbors. In light of these constraints, the deformation of an HCP polycrystal must occur via mechanical twinning to avoid cracking at the grain boundaries.

The dislocation sources in crystal grains are continuously induced in the near-surface of specimens due to the shear stresses. The dislocation density increases gradually, and many dislocation pile-ups form. When plastic deformation occurs, deformation twinning is induced at the location of the dislocation block due to the low number of slip systems. Impact waves caused by the collapse of a cavitation bubble can produce significant strain, a high strain rate, and numerous direction cycle loads, which all induce the overlapping and interaction of deformation twinning. This indicates that the enhancement mechanism of WCP might be related to the activity of the deformation twinning and the high density of dislocations. At the same time, the evolution of microstructures can also induce compressive residual stress in the near-surface of the specimens.

From the results in this paper, we conclude that the mechanism corresponding to the model proposed in this paper is appropriate. Since it accurately describes the systems investigated here, we feel it may be useful for designing WCP process conditions, and perhaps for harnessing the possible reinforcing effect observed in the WCP-processed specimens.

Fig. 3: The microstructural evolution process of pure titanium with WCP duration, at the same observation point.
Fig. 4: OM microstructures at a depth of 30-40 μm from the surface.

Fig. 5: TEM microstructures at a depth of 30-40 μm from the surface. (a) The interaction of deformation twinning in two different directions, as well as the high density dislocations among the bands of twinning ; (b) Three types of twinning systems cross at the same point.

Table 2 : The hardness changes induced by WCP on the surface

| Process     | Vickers hardness (HV) | Average (HV) |
|-------------|-----------------------|--------------|
| Unpeened    | 148 147 160 147       | 156          |
| Peened      | 165 160 175 170       | 173          |
4. Conclusions
The results obtained in this investigation show that WCP can induce a stable compressive residual stress in the superficial layer of titanium specimens. The depth of the compressive residual stress zone can be up to approximately 150 μm. Deformation twinning and dislocations play an important role in the micro-plastic deformation of HCP-structured metal materials.

The following conclusions can be drawn from this paper concerning the residual stress generation mechanism. The dislocation density of the α-phase of pure titanium increases when the impact energy caused in the WCP process exceeds the internal energy of the pure titanium crystal in the initial WCP process stages. This was confirmed to generate twinning deformation via the dislocation-induced formation and development of a slipping zone. The deformation due to twinning, the interaction between these deformation twins and dislocations, and local micro-plastic deformation are all induced by WCP in the strengthening layer. These findings indicate that the enhancement mechanism of WCP might be related to both the activity of the deformation twinning, and to the dislocations. The predicted results of residual stress in the near-surface of pure titanium were in good agreement with those of the experimental measurements.
Acknowledgements

This research receives ongoing support from the High-Tech Research Center and Open Research Center at the Saitama Institute of Technology.

References

[1] Hammitt FG and De MK. 1979 Wear 52 243-262
[2] Tomita Y and Shima A 1986 J. Fluid Mech. 169 535-564
[3] Chen YL, Kuhl T and Israelachvili J 1992 Wear 153 31-51
[4] Sun Z, Kang XQ, Wang XH 2005 Mater. Des. 26 59-63
[5] Tang CH, Cheng FT and Man HC 2006 J Surf. Coat. Tech. 200 2602-2609
[6] Qin M, Ju DY and Oba R 2006 Surf. Coat. Tech. 200 5364-5369
[7] Han B, Ju DY and Jia WP 2007 Appl. Surf. Sci. 253 9342-9346
[8] Sahaya Grinspan A and Gnanamoorthy, R., 2006 Appl. Surf. Sci. 253, 989-996.
[9] Sahaya Grinspan A and Gnanamoorthy R 2006 Appl. Surf. Sci. 253 997-1006
[10] Sahaya Grinspan A and Gnanamoorthy R 2006 J Surf. Coat. Tech. 201 1768-1775
[11] Ramulu M, Kunaporn S, Jenkins M, Hashish M and Hopkins J.2002 J. Press. Vess. Technol. 124 118-123
[12] Kunaporn S, Ramulu M, Jenkins M and Hashish M 2005 J. Press. Vess. Technol. 127 186-192
[13] Sahaya Grinspan A and Gnanamoorthy R 2007 J. Manuf. Sci. Eng. 129 601-606
[14] Sahaya Grinspan A and Gnanamoorthy R 2007 J. Eng. Mater. Technol. 129 609-613
[15] Han B, Ju DY and Nemoto T 2007 Mater. Sci. Forum 561-565 2485-2488
[16] Ju DY, Qin M, Koubayashi T and Oba R 2006 Surf. Eng. 22 219-223
[17] Qin M, Ju DY and Oba R 2006 Surf. Coat. Tech. 201 1409-1413
[18] Martin U, Altenberger I, Scholtes B, Kremmer K and Oettel H 1998 Mater. Sci. Eng. A 246 69-80
[19] Altenberger I, Scholtes B, Martin U and Oettel H 1999 Mater. Sci. Eng. A 264 1-16
[20] Wu X, Tao N, Hong Y, Xu B, Lu J and Lu K 2002 Acta Mater. 50 2075-2084
[21] Harada Y, Fukaura K and Haga S 2007 J. Mater. Process. Tech. 191 297-301
[22] Wang TS, Lu B, Zhang M, Hou RJ and Zhang FC 2007 Mater. Sci. Eng. A 458 249-252
[23] Noyan C and Cohen JB, 1987 Residual Stress Measurement by Diffraction and Interpretation, Springer-Verlag, New York, pp. 2-101
[24] Ju DY 2002 Handbook of Residual Stress and Deformation of Steel. In: Totten G, Howes M and Inoue T (Eds.), ASM International, Ohio, pp. 372-398
[25] Meyers MA, Vöhringer O and Lubarda VA 2001 Acta Mater. 49 4025-4039
[26] Gilman JJ 1997 Phil. Mag. 76 329-336
[27] Jordan AS, Caruso R and von Neida AR. 1980 Bell Syst. Tech 59 593-637