Journal of University of Science and Technology Beijing
Vol.6(1999), No.1, p.64

A New Method for Fractal Dimension Determination by STM at Nanometer Scale

Qikai Li [1], *Yue Zhang*[1], *Wuyang Chu*[1], *Chen Wang*[2], *Chunli Bai*[2]

1) Applied Science School, University of Science and Technology Beijing, Beijing 100083, China
2) Chemical Institute, Chinese Academy of Science, Beijing 100080, China

(Received 1998-10-16)

Abstract: A new method for determining the fractal dimension by STM at nanometer scale has been proposed. Weierstrass-Mandelbrot fractal curves were used to verify the accuracy and reliability. The Computer simulation showed that the fractal dimension obtained with this method generally outran the traditional yard method. The new method has been applied to the fractal dimension determination of the fractures of Ti_3Al and Ti-24Al-11Nb alloys. The results show that the fractal dimension of Ti-24Al-11Nb alloy is higher than that of Ti_3Al, and it varies with the crack extending orientation.

Key words: fractal dimension; STM; nanometer scale; Ti-Al alloy

In recent years, many authors have used Slit Island Method (SIM) in the fractal dimension determination of fractured surface, which is fulfilled by measuring a series of parameters, such as perimeter-maximum diameter, perimeter-area. The determination of fractal dimension by perimeter-area relation is first used by Mandelbrot *et al.* [1] in fractured specimens of steels. Later on, much work has been done on the use of the method in determining the fractal dimensions of fractured surfaces [2, 3], and on the fractal study of grain structure, fatigue erosion pits, inclusions *et al.* [4, 5]. On the basis of the work of Mandelbrot *et al.* and the consideration of limited nesting of natural fractals, Lung *et al.* proposed a method for determining the fractal dimension by employing the perimeter-maximum relation [6, 7].

As to the fractal dimension evaluation of vertical sections, various measuring methods have been devised, such as box-counting method, yard method and power spectrum method. However, owing to the difference of various dimension determination methods, not all methods yield satisfactory results. Especially in nanometer scale range, because of the limitation of experimental method, nanometer scale fracture analysis poses a challenge. The authors have used the scanning tunneling microscope (STM) in the fractal dimension study of metallic composite fractures by employing a new method [8], however, theoretical study has not been done. In this article, the method will be discussed from a theoretical point of view, and thus a new ground for STM application in fractal study at nanometer scale is opened. We define the new method as the varying instrumental resolution.

1 Principle of the method

According to Mandelbrot [1], the total length $L(\varepsilon)$ of the fractal curve is

$$L(\varepsilon) = \varepsilon^{1-D},\ L(1) = 1 \qquad (1)$$

Suppose absolute yard is η, the initial shape length (or upper limit of self-similar structure) is L_0, then

$$L(\eta) = L_0^D \eta^{1-D} \qquad (2)$$

$$\log L(\eta) = D\log L_0 + (1 - D)\log\eta \qquad (3)$$

There exist multiple methods in determining D:

(1) fix L_0, find D by changing η, which results in the so-called Richardson method.

(2) fix η, find D by changing L_0, which results in the perimeter-maximum diameter method [6, 7].

(3) fix measuring range, find D by changing η realized indirectly by STM, which thus results in our method.

In order to use the method, first, the measuring range has to be fixed, a set of data is thus obtained by STM; later on, the fractal dimension is calculated from the slope of the regression line according to equation 3.

2 Computer simulation

In order to evaluate the stability and reliability of the method by varying instrumental resolution, computer simulation has been done on Weierstrass-Mandelbrot (WM) curves. The WM function [7] is given as

$$f(x) = \sum_{n=-\infty}^{\infty} b^{-nH}(1-\cos b^{n}x) \qquad (4)$$

where the constant $b>1$, the Hausdorff dimension H is between 0 and 1, and the local dimension D equals $2-H$.

The typical WM curves are illustrated in **figure 1.**

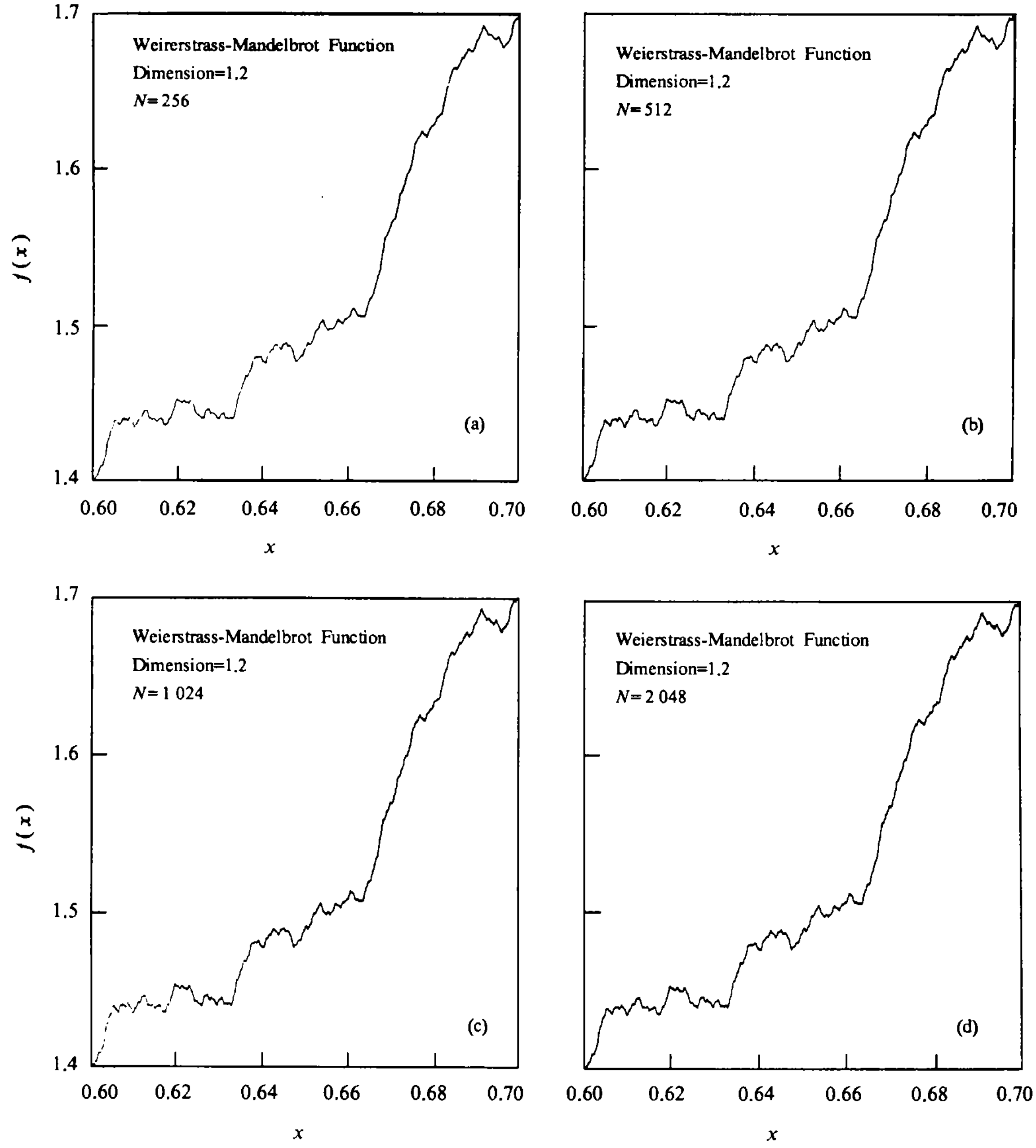

Figure 1 Profiles of WM curves with the same local dimension ($b=2.1$) and different point number N

More details can be seen as the point number N increases, the profiles are analyzed in the same manner as those extracted from the experimentally acquired STM images. Therefore, the comparison between the conventional yard method and the method by varying instrumental resolution could be done on standard WM profiles. The point number N used in the conventional yard method is 8 192. The point number series for the method by varying instrumental resolution is 256, 512, 1 024, 2 048, 4 096 and 8 192. The typical plot for measuring fractal dimension with the method by varying instrumental resolution is shown in **figure 2**, while the results for various theoretical dimensions with yard method and our new method are displayed in **figure 3**. As shown in figures 2 and 3, the results gained by our method are superior to those determined by the conventional yard method, and the values corresponding to different point number N all lie in the same line, which indicates that very limited number of experimental points could score satisfactory results in practice.

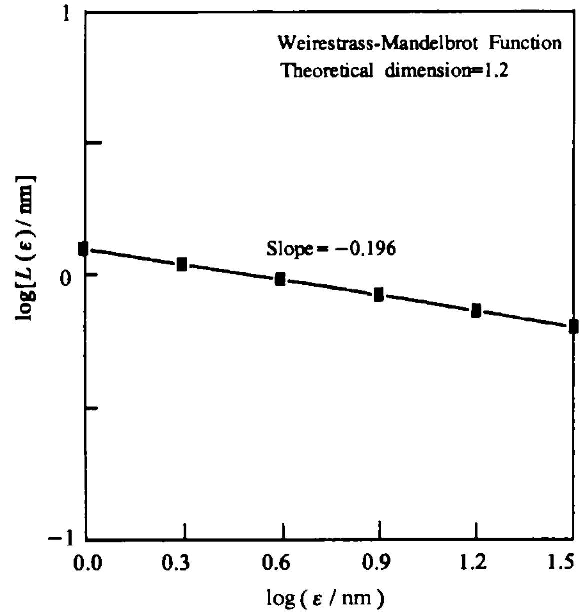

Figure 2 Result calculated with method by varying resolution on WM profiles (b=2.1) of the same local fractal dimension

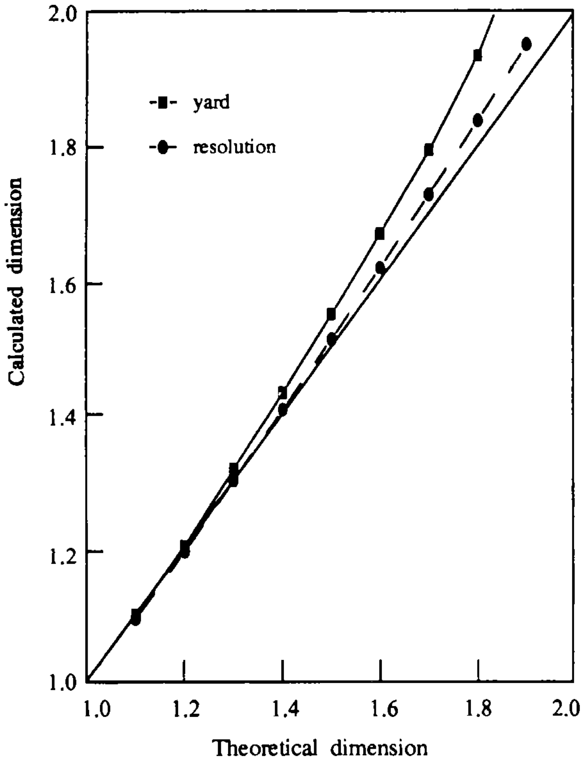

Figure 3 Comparison of results calculated with conventional method and with method by varying resolution on WM profiles(b=2.1) of various local fractal dimensions

3 Experiment and results

The fractured surfaces of alloys Ti$_3$Al and Ti-24Al-11Nb were observed with STM by using constant-current mode. Various STM images were scanned by using different pixel numbers as to the same scan range of the above-mentioned alloys, which is equivalent to selecting different yards, thus, the images with various details could be obtained. The features of STM images are enriched with the increasing of pixel number, *i. e.*, the decrease of measuring yard ε, and thus that of 3D STM image could better represent the real roughness of fractured surface.

By selecting different pixel numbers, *i. e.* different yard ε, the same range of the fractured surface was scanned, and thus a set of STM images and their corresponding 3D views of fractured surface with different resolutions were obtained. The length $L(\varepsilon)$ of the profile corresponding to different ε was calculated by computer directly or measured with image analysis instrument, the plot of $\ln L(\varepsilon)$-$\ln\varepsilon$ was drawn and the fractal dimension D was calculated with linear regression. In order to increase the accuracy, multiple vertical profiles for each image were adopted.

The typical STM images with the same scan range are illustrated in **figure 4**. The change of $\ln L(\varepsilon)$ with $\ln\varepsilon$ along different directions as to the notched tip of the fractured surface of alloy Ti$_3$Al, such as, X direction (along the crack extending direction, curve 1), Y direction (perpendicular to the crack extending direction, curve 2) and XY direction (45 ℃ from X direction, curve 3), are shown in **figure 5**. The change of $\ln L(\varepsilon)$ with $\ln\varepsilon$ along different directions as to the notched tip of fractured surface of alloy Ti-24Al-11Nb, such as, X direction (curve 1), Y direction (curve 2) are shown in **figure 6**.

Experimentally, in order to improve the accuracy, multiple profiles along the same direction were averaged. As shown in figures 5 and 6, good linearity of $\ln L(\varepsilon)$ with $\ln\varepsilon$ of the above-mentioned alloys was maintained at a nanometer scale, thus the fractured surfaces of alloys Ti$_3$Al and Ti-24Al-11Nb possess the fractal characteristics.

The fractal dimensions were calculated from the $\ln L(\varepsilon)$-$\ln\varepsilon$ relationship, the results are shown in **table 1**, and the apparent fracture toughness of alloys Ti$_3$Al and Ti-24Al-11Nb are also listed in table 1.

At micrometer scale, the fractal dimension D of the fractured surfaces of Ti-24Al-11Nb along the crack extending direction was 1.203, while that of the fractured surfaces of Ti$_3$Al was 1.081 [9], which corresponds to micro-scale cleavage steps in microstructure. However, at nanometer scale, the fractal dimensions of the two alloys differ from those at micrometer scale, which in turn correspond to nano-scale cleavage steps. Different dimension corresponds to different measuring space, which is in agreement with the multi-

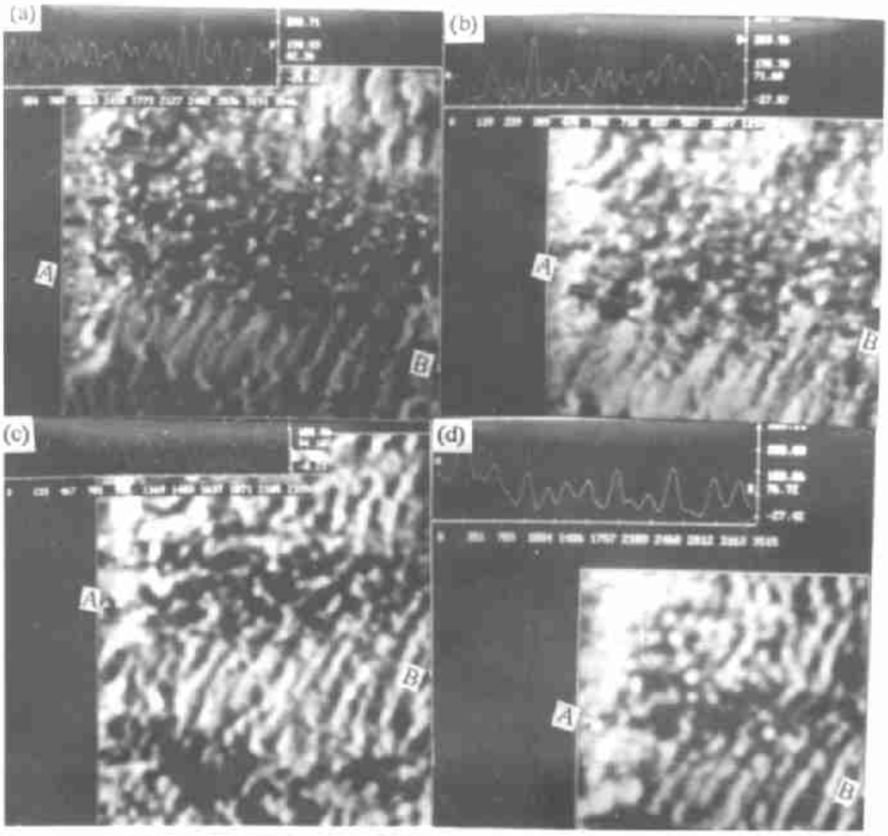

Figure 4 STM images and profiles of fractured surfaces with different scan pixel numbers, scan range is 820 nm×976 nm. (a) 180×180. (b) 150×150. (c) 120×120. (d) 90×90 pixels.

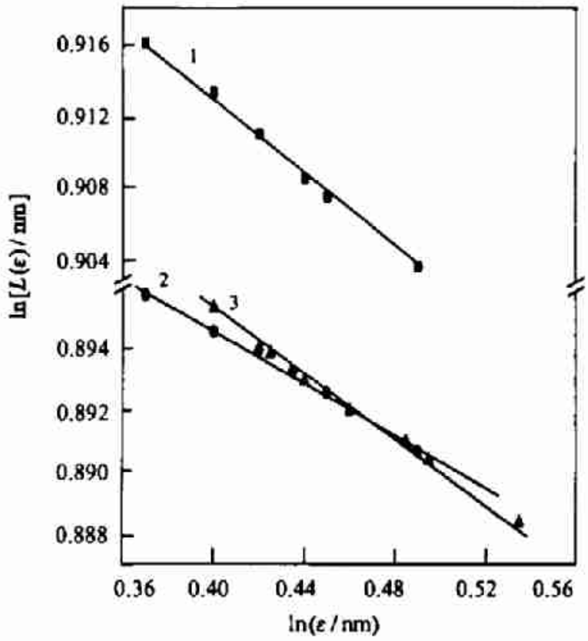

Figure 5 Plot of $\ln L(\varepsilon)$-$\ln\varepsilon$ for fractured surfaces of alloy Ti_3Al measured with STM, 1—*X* direction, 2—*Y* direction, 3—*XY* direction

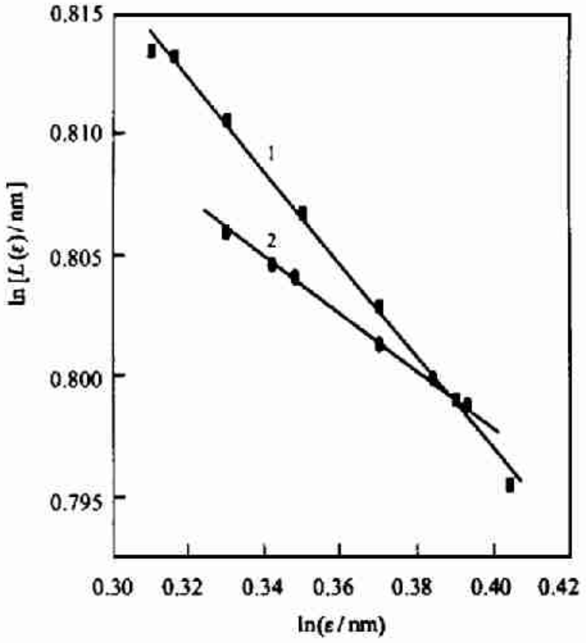

Figure 6 Plot of $\ln L(\varepsilon)$-$\ln\varepsilon$ for fractured surfaces of alloy Ti-24Al-11Nb measured with STM

Table 1 Fractal dimensions along different scan directions of fractured surfaces of alloys

Alloy	K_{IC} / MPa·m$^{1/2}$	D_X	D_Y	D_{XY}
Ti_3Al	9.6	1.092	1.046	1.055
Ti-24Al-11Nb	20.0	1.172	1.083	—

range fractal theory proposed in [10].

4 Conclusions

It is applicable to use STM for fractal dimension determination at nanometer scale. The results gained by the method of varying instrumental resolution are superior to those obtained by the conventional yard method. Because of its simplicity and accuracy, the method could be easily adopted in practice.

Acknowledgment

This work was supported by the National Natural Science Foundation of China and the Basic Science Foundation of the Metallurgical Ministry of China.

References

[1] B.B. Mandelbrot: *The Fractal Geometry of Nature*, Freeman, San Francisco, 1983, p. 25, 29, 459.

[2] B.B. Mandelbrot; D.E. Passoja; A.J. Paullay: *Nature*, 308 (1984), p. 721.

[3] J.Y. Zhang; S. Zhu, *et al.*: *Acta Metallurgia Sinica*, 12 (1992), No. 28, p. 530.

[4] X.G. Jiang; J. Cui; Z.L. Ma: *Adv. in Mat. Sci.*, 4 (1991), No. 5, p. 315.

[5] Y. Zhang; Z.H. Wang; W.Y. Chu, *et al.*: *Science in China*, A25 (1995), No. 6, p. 659.

[6] C.W. Long; Z.Q. Mu,: *Science in China*, A24 (1994), No. 1, p. 94.

[7] P. Pferifer: *Appl. of Surf. Sci.*, 18 (1984), p. 146.

[8] Y. Zhang; W.Y. Chu; Y.B. Wang, *et al.*: *J. Vac. Sci. Technol. B*, 12 (1994), No. 3, p. 1722.

[9] Y. Zhang; W.Y. Chu; Y. Wang, *et al.*: *Acta Metallurgia Sinica*, A29 (1993), No. 9, p. 393.

[10] C.W. Lung: *Mater. Sci. and Eng.*, A177 (1994), p. 299.

[*continued from page* 63]

preferred orientation, which results larger amount of deposit building upon the die face during forming. It was interesting to find that ($00X$) plane preferred orientation of the zinc crystal tended to be increasing when the deposit was performed in forming deformation owing to the rotating of the crystalline grains, which deteriorates the forming conditions.

Acknowledgments

Authors are indebted to Mr. Zheng Jianping, of Bao steel group (Shanghai, China), for his helpful comments and providing for the IF sheet steel bases. Financial support of our work is from National 9th Five-year Project of China, and from the Open Laboratory of Corrosion, Abrasion & Surface Technology of the Former National Metallurgy Department, which is highly acknowledged.

References

[1] Hisashi Hayash; Takeo Nagawa, *et al.*: *J. mater. pro. Technol*, 46 (1994), p. 455.

[2] J.H. Lindsay; R.F. Paluch, *et al.*: *Plating & Surface Finishing*, March (1989), p. 62.

[3] J.H. Lindsay; R.F. Paluch, *et al.*: *Plating & Surface Finishing*, May (1992), p. 129.

[4] Jun Hisamoto; Kouki Ikeda, *et al.*: [In:] *The Minerals, Metals & Materials Society*, George Krauss, K. David Matlock [eds.:] , 1990, p. 331.

[5] Y. Lu: *Anticorrosion Treatment on Metal Surface*, Metallurgical Industry Press (in Chinese), Beijing, 1995.

[6] Woong-Chul Shin; Soon-Gil Yoon: *Electrochem. Soc.*, 144 (1997), p. 1055.

[7] Mitsutosh Sakaguchi; Shigeki Kirihara, *et al.*: *Surface Technology* (Japanese), 33 (1982). p. 67.

[8] S.J. Shaffer: [In:] *Proceeding of the International Conference on Zinc and Zinc Alloy Coated Steel Sheet* (*GALVATECH*), The Iron and Steel Institute of Japan, Tokyo, 1989, p. 338.