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REVIEW PAPER

ELEMENTAL DETERMINATION OF A SOLID SURFACE BY THE LOW ENERGY ION SCATTERING TECHNIQUE

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Abstract

Several methods can be used to determine the elemental composition and surface structure of solid materials. Among more accurate ones, there is a method of using the low energy ion scattering technique (LEIS). Owing to the sensitivity of this technique when applied to the top-most surface layers, it is considered an ideal method among other surface techniques. The LEIS technique supplies useful information about the composition, concentration and surface structure of metals and metal alloys. Mono-energetic ions such as helium with low energies are used to analyze surfaces. By using computer simulation, elements in solid bulk as well as on the surface of a solid body could be determined. In this study, the SABRE computer code was used for this purpose. The LEIS technique is based on energy transfer between incident ions and target atoms. It is necessary to have certain information such as the incident and azimuthal angles as well as the incident energy in order to perform this type of scattering. The application of the LEIS technique generates an energy spectrum, which was the purpose of the present work. This spectrum is achieved from simulation data which present certain peaks. Once the peaks are analyzed, masses of elements on the surface and hence the structure type could be determined by the energy difference between incident and scattered ion beam energies and the peak counts. The sample used in this project was Al- Pd- Mn quasicrystal. Three relatively clear peaks appeared for the sample representing consistent elements. The results proved that all the three elements, Al, Pd and Mn, were present on the surface.

Keywords: surface composition, simulation computer, Al, Pd and Mn elements, Low Energy Ion Scattering (LEIS).

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INTRODUCTION

Surface studying techniques have been developed over the recent years to determine properties of solids. An example is the ion microprobe method (Honig 1958, Bradley 1959, Stanton 1960, Bradley et al. 1960, McHugh et al. 1964, Woodyard et al. 1964, Liebl et al. 1963, Smith et al. 1963), in which a surface is studied by ion bombardment and scattered particles are analyzed by a mass spectrometer. An analysis of elastically scattered primary ions in order to determine surface composition was first performed by Rubin (1959) in a study in which primary ion energies were relatively destructive (in the MeV range). Each peak in the energy spectrum of scattered ions corresponds to scattering from a different species of the target atom. Later, Panin (1962) using 10-100KeV ions, and Datz and Snoek (1964) using 40-80 keV Ar+ ions found that binary elastic collisions were predominant with the scattered ions having energies estimated by the simple binary elastic collision theory.

The Low Energy Ion Scattering (LEIS) method is useful for analyzing solid surface. This technique can answer questions such as which elements exist on the surface, how much of each element there is on the surface and where the elements are located. Mono low-energy ions are used in this technique to analyze the surface (Samavat et al. 2007). A low energy ion beam is emitted to the surface atoms and then is scattered from these atoms. This technique was first used in 1968 by Smith to study some metal surfaces (Smith 1967). The LEIS is remarkably useful for studying the structure and composition of surfaces of metals and alloys (O'Connor et al. 2003). This technique is one of the Ion Scattering Spectroscopy methods which provide information about the composition and structure of surface layers (Niehus et al. 1992, Taglauer, Vickerman 1997). The resulting energy loss, for each binary elastic collision, depends on the mass of the target atom and the scattering angle, θ (Smith 1967, Williams, Rabalais 1994, Goebl et al. 2015). The ions' energy range used in the present work is 100 eV to 10 keV (Samavat et al. 2007).

The LEIS technique is based on energy transfer between incident ions and target atoms; and if the mass of a target atom is near to the mass of an incident ion, this transfer is much greater. To study the surface composition, elements on the surface should be determined. Information about surface composition can be obtained from energy spectra of the scattered ions.

The LEIS technique consists of directing a beam of mono-energetic ions to a surface and measuring the kinetic energy of the scattered ions (Smith 1967, Bastasz et al. 2000). Mono-energetic ion beams are emitted to the surface and interact with the surface atoms; by using the angular distribution and energy of scattered ions from surface atoms, masses of surface atoms can be determined.

The LEIS is a quantitative technique that is uniquely sensitive to the elemental composition of the topmost surface layer. With a combination of subsurface layers' shadowing and high neutralization probability of the incident and scattered light noble gas ions, the very top atomic surface layer only could be measured (Samavat et al. 2011, Samavat et al. 2008). LEIS measurements provide information about the channeling surface composition of an Al-Pd-Mn sample after sputtering and annealing. Using 2 KeV He+ and Ne+, the Al and Mn surface concentrations were determined under bombardment (Samavat et al. 2008). The SABRE computer code was used to obtain the energy spectrum from simulations. In this study, types of atoms on the surface and thus the surface composition were determined by using the energy spectrum of a quasicrystal,.

DETERMINATION ON THE SURFACE

The identification of atoms in the surface layer is the simplest form of a compositional analysis using the LEIS. The procedure involves the acquisition of an energy spectrum of ions, normally inert gas ions, scattered off the surface when the projectile mass, incident energy and scattering angle are known (Samavat et al. 2007). The scattered energy peaks are then compared with those given by relation E/E_0 according to θ, to reveal the target atom mass (O'Connor, MacDonald 1990).

In the LEIS, a mono-energetic beam of inert gas or alkaline ions are emitted and then collide with target atoms, whereupon projectiles are scattered and can be detected by a detector. These scatterings occur elastically. Having identified the energy spectrum, the mass of a target atom can be determined by scanning the surface. Using the information from the detector, the energy spectrum which contains specific peaks will be gained.

Energies related to the peaks are energies of ions scattered off the surface and by the use of this energy E_0 and Eq. 1 masses of surface atoms and therefore atomic species can be determined. Consider collision between a projectile with mass m_1, velocity v_0, energy E_0, and a target atom with mass m_2, which was initially at rest (Samavat et al. 2007). After the collision,

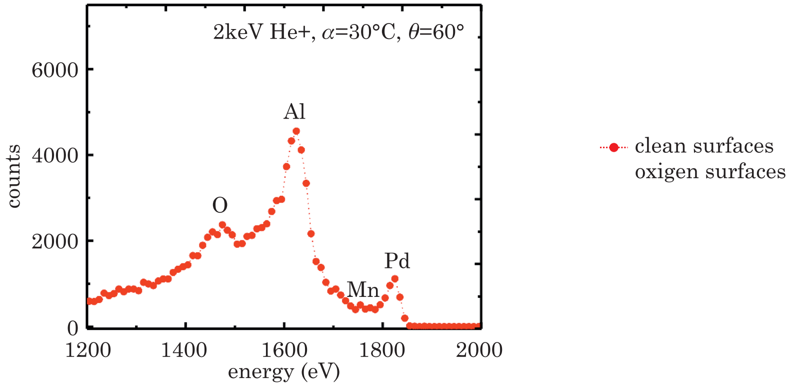

Fig. 1. Energy spectrum of 2 keV He+ ion scattered from a quasicrystal surface

the projectile and the target atom have velocities v_1 and v_2. Applying the energy and momentum conservation principle (O'CONNOR et al. 2003), we have

$$\frac{E_f}{E_0} = \left(\frac{\cos\theta + \sqrt{\mu^2 + \sin^2\theta}}{1+\mu}\right)^2 \tag{1}$$

where, E_0, E_f are projectile energy before and after collision, θ is the scattering angle and µ is the ratio of the target atom mass over the projectile mass (). Thus, having these parameters at hand, the mass of the target atom can be measured and the atoms on the surface can be detected. For better detection, it is advisable to use a projectile with a mass as close as possible to the mass of a target atom, and also to employ the largest possible scattering angle (O'CONNOR et al. 2003, GLADYS et al. 2004). Figure 1 shows energy spectra of He+ ions scattered from an Al-Pd-Mn quasicrystal surface at the scattering angle of 30°. Peaks of this energy spectrum are the result of He+ ions colliding with the surface atoms.

Figure 2 demonstrates that scattering signals become more intense at smaller θ. However, the energy separation between the various scattering peaks narrows as θ decreases. A compromise between the signal strength and peak separation is necessary and the experiments have indicated that θ=75° provides satisfactory results, as shown in Figure 1.

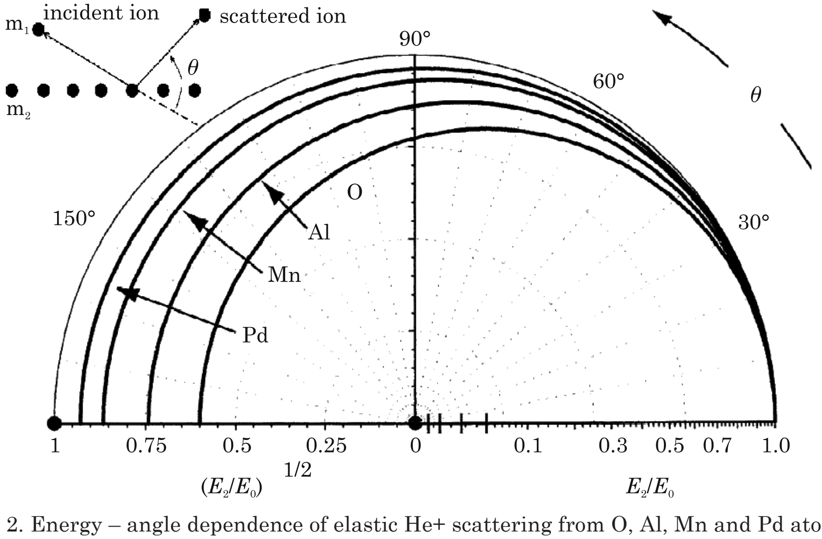

Fig. 2. Energy – angle dependence of elastic He+ scattering from O, Al, Mn and Pd atoms displayed as a polar plot with E_1/E_0 as the radial coordinate and the laboratory scattering angle θ as the angular coordinate

The curves are circles that pass through the point (1,0°) according to Eq. 1 and illustrate how mass resolution increases with θ (BASTASZ 2002).

$$U(r) = \frac{Z_1 Z_2}{r}\varphi({r}/{a}) \tag{2}$$

where Z_1 and Z_2 are the atomic numbers of incoming ions and the target atoms, r is the separation of the nuclei, and a is the screening length.

A number of different screening functions and screening lengths have been proposed. The two most widely used are the Moliere potential applied to the Thomas-Fermi model of the atom TFM – (MOLIÈRE 1947), and the universal potential (ZBL) – BIERSACK et al. (1982). The ZBL potential has been shown to be the best fit to the range of currently available measurements of the interatomic potential. We can approximate closely the motion of the scattered ions and the recoil target atoms by calculation based on this repulsive interaction. The signal intensity which is shown in Figure 1 can be calculated using screened Coulomb potentials (ZIEGLER, BIERSACK 1985).

One common method applied to surface composition analysis is the use of reference material as a standard. Consider elements A and B which have surface concentrations N_A and N_B, respectively. The scattering yield from each element is proportional to the amount of the target element on the surface. The scattering yield from A and B atoms, Y_A and Y_B, can be related to the atomic concentrations by

$$\frac{Y_A}{Y_B} = S\frac{N_A}{N_B} \tag{3}$$

The theory of scattering two point charges was first published by THOMSON (1903). When a low energy ion approaches a target atom at a surface, the nuclei will repel each other and the projectile will be scattered. The interatomic potential is described as a modified or screened coulomb-potential with a screening function $\Phi(r/a)$.

Whereas S is called the relative sensitivity factor of element A to element B, and it includes relative cross sections and charge fractions. If experimental measurements are performed with standard samples of pure A and pure B under the same conditions as those for the alloy, and one makes the assumption that the charge fraction is not composition dependent, the value of the sensitivity factor for the two elements, A and B, can be obtained (O'CONNOR et al. 2003, SAMAVAT et al. 2007). If only A and B are present, then we have

$$N_A + N_B = 1 \tag{4}$$

The SABRE computer code was used to obtain the energy spectrum. This program simulates interactions by following the projectile trajectory in the crystal. Applying the input data, the program was run for a quasicrystal at the azimuthal angle φ=180°, incidental angle α=20° and the exit angle β=130° using 1 keV He+ particles.

After running the program, the outputs were analyzed in Excel program, producing the energy spectrum for φ=180°; the results are shown in Figure 2.

By entering the energy amounts in Eq. 1 and knowing He mass, masses of target atoms on the surface are computable.

Having the scattering, incident and azimuthal angles and also knowing the incident energy, energy spectra can be given. Output data which were measured with the Maple program for θ=60°, α=20°, φ=180° and E_0=1 keV, are discussed in this section. Finally, the energy spectrum which gives the ratio E_f/E_0, was drawn and μ from Eq. 1 was obtained for the spectra; comparison of the mass of each element on the surface to the helium mass can be based on the energy spectra, as shown in Table 1. The data prove that elements on the surface comprise Al, Pd and Mn.

Table 1

Masses of Al, Mn and Pd of a quasicrystal by simulation

Element	Mass (kg)
Al	4.32×10^{-26}
Mn	8.64×10^{-26}
Pd	16.9×10^{-26}

Values in Table 1 are achieved from the relation of the energy of every element on the surface, shown in Figure 3, to the mass of a helium ion (6.4×10^{-27} kg).

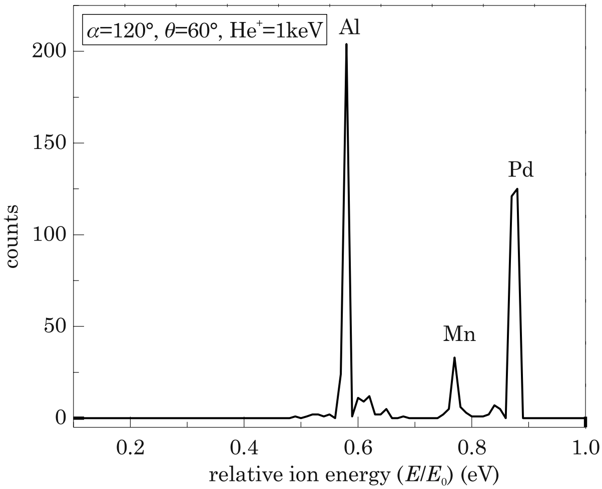

Fig. 3. Energy spectrum gained by simulations

The low energy ion scattering technique provides useful information about the composition, concentration and structure of the surface of metals and metal alloys. To study surfaces, mono-energetic ions such as helium with low energies are analyzed. These ion beams are emitted to the surface and are then scattered from the surface atoms. In our study, the energy spectrum was given using the SABRE computer code. With the input data, this program was run at the azimuthal angle 180°, incident angle 20°, exit angle 130° and 1 keV He+ as the probe particle. After running the simulations, the output was analyzed in Excel program and the energy spectra gained for the azimuthal angle (φ=180°) were obtained.

Due to the Helium mass one can get mass of each element on the surface from the energy spectra, and in this way surface elemental composition of the material and also concentration of the materials on the surface can be determined. As what got from the outputs there were Al, Pd and Mn elements on the surface.

CONCLUSION

The purpose of this study was to determine elements on an Al-Pd-Mn quasicrystals surface. We have used the low energy ion scattering technique for obtaining useful information in order to analyze the composition of quasicrystal surfaces. By using computer simulation, the elements and structure of a solid surface were determined.

Our findings suggest that there were three types of elements on the surface, determined from the energy spectrum gained from simulation data that had certain peaks and from elemental masses. The sample used for this project is an Al-Pd-Mn quasicrystal. Demonstrably, three relatively clear peaks (Al, Pd, Mn elements) appeared in the spectrum, which represented the three consistent atom types.

AKNOWLEGMENT

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