زانكۆی سەلاحەدین - هەولێر
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INVESTIGATION OF THERMAL EXPANSION IN SILICON AND COPPER

Research Project

Submitted to the department of Physics in partial fulfillment of the requirements for the degree of BSc. in Physics

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بِسْمِ اللَّهِ الرَّحْمنِ الرَّحِيمِ

قَالُواْ سُبْحَانَكَ لاَ عِلْمَ لَنَا إِلاَّ مَا عَلَّمْتَنَا إِنَّكَ أَنتَ الْعَلِيمُ الْحَكِيمُ

صدق الله العظيم

سورة البقرة الاية32

Supervisor Certificate

This research project has been written under my supervision and has been submitted for the award of the degree of BSc. in (Physics).

Signature
Name Dr. Ayoub Sabir Karim
Date 6 / 4 / 2023

I confirm that all requirements have been completed.

Signature:
Name: Rashad Hassan Mahmud
Head of the Department of Physics
Date / /

This project is dedicated
to:

Allah Almighty, my
Creator and my Master,

My great teacher and
messenger, Mohammed
(May Allah bless and
grant him), who taught us the purpose of life,

My homeland Kurdistan, the warmest womb,

The Salahadin University; my second magnificent home;

My great parents, who never stop giving of themselves in countless ways,

My beloved brothers and sisters;

To all my family, the symbol of love and giving,

My friends who encourage and support me,

All the people in my life who touch my heart.

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SUMMARY

In this research project we will focus on thermal expansion of Solids, Solid materials expands very less as compered to liquid and gases. Gases expands much more than liquid and solids. This happens because intermolecular force of attraction is very strong in solids, intermediate in liquids and very weak in case of gases.

The linear thermal expansion coefficients of single-crystal silicon have been determined in the temperature range 293 to 1000 K using a dilatometer which consists of a heterodyne laser Michelson interferometer and gold versus platinum thermocouple. The present data are compared with the data previously obtained by similar dilatometers and the standard reference data for the thermal expansion coefficient of silicon, recommended by the Committee on Data for Science and Technology (CODATA).

Also Measurements of the thermal expansion of copper (NBS Standard Reference Material, SRM736) have been made between 300 and 700 K. Agreement with the NBS calibration was obtained up to 630 K within 0.5 %, but at 700 K the difference amounted to 2.5%.

CHAPTER ONE

INTRODUCTION

1.1 Introduction

‘Solid State Physics’. As the name suggests, is the study of rigid matter, through methods such as quantum Mechanics, crystallography, electromagnetism, and metallurgy, and it is the largest Branch of condensed matter physics. Solid state physics studies how the large-scale Properties of solid material result from their atomic-scale properties and form a Theoretical basis of materials science. Solid is one of the four fundamental states of matter (the others being liquid, gas, and plasma). The molecules in a solid are closely packed together and contain the least amount of kinetic energy. A solid is characterized by structural rigidity and resistance to a force applied to the surface. Unlike a liquid, a solid object does not flow to take on the shape of its container, nor does it expand to fill the entire available volume like a gas. The atoms in a solid are bound to each other, either in a regular geometric lattice (crystalline solids, which include metals and ordinary ice), or irregularly (an amorphous solid such as common window glass). Solids cannot be compressed with little pressure whereas gases can be compressed with little pressure because the molecules in a gas are loosely packed [Simon, 2013].

1.2 Types of Solids

The different structures that solids possess can be divided into two main types. (Crystalline solids and Amorphous solids) crystalline solids are composed of a regularly repeating pattern of atoms, amorphous solids have structures in which the arrangement of atoms is much more random. The physics of amorphous materials is less well understood, and more complicated, than that of crystalline materials.

Crystalline solids are made up of atoms arranged in a 3-D pattern that repeats itself again and again throughout the entire solid. The way in which the atoms are arranged is known as the crystal structure

Examples of Crystalline solids :

1. Diamonds
2. Ice
3. Potassium chloride

In nature, crystalline solids rarely appear in their pure form. Most often, they are found as polycrystalline solids. This means that they grow in the form of lots of little crystals known as “crystallites” or “grains,” which vary in size and point in different directions with respect to each other.

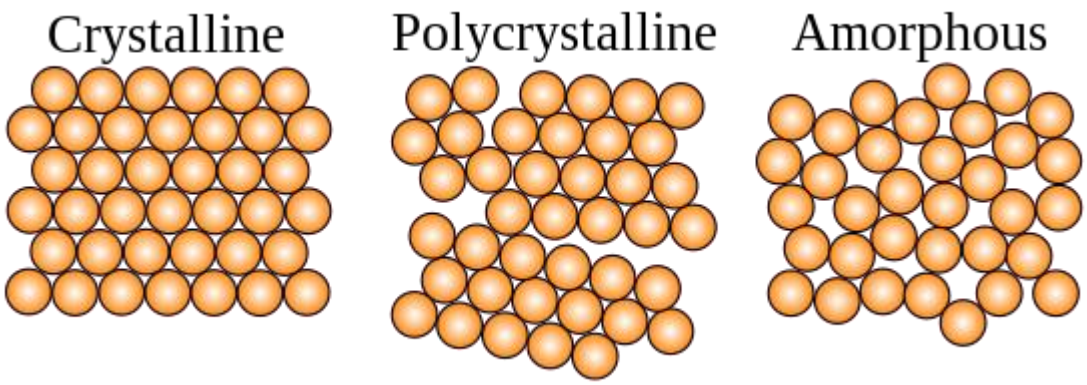
Examples of Polycrystalline solids :

1. Common metals
2. Most ceramics
3. Glass ceramics

Although many solids are crystalline, there are also plenty that are amorphous. The word “amorphous” comes from both the Latin and Greek words for “shapeless,” and is generally taken to mean something without an organized structure. Despite having this label, the atoms are not in fact completely randomly arranged in amorphous materials. However, they are arranged in a more random way than the atoms of a Crystalline solid [Holgate, 2021].

Examples of Amorphous Solids :

1. Glass
2. Rubber
3. Plastics



1.3 Solid Material Expansion

Most materials increase their volume as the temperature T is raised. Since also the thermal displacement of atoms increases, one might think that the atoms “push” their neighbours apart. However, this is a misleading argument. A crystal described with perfectly harmonic lattice vibrations

shows no thermal expansion at all. Many solids, for instance silicon and germanium and some alkali halides, shrink with increasing T, at low temperatures. Some solids with non-cubic lattice structures, for instance zinc and uranium, shrink in one direction but expand in others so that there is a net volume increase. There are also materials, such as invar alloys, which have a very small or slightly negative coefficient of thermal expansion at ambient temperatures [Grimvall, 1999]. Thermal expansion is the phenomenon observed in solids, liquids, and gases. In this process, an object or body expands on the application of heat (temperature). Thermal expansion defines the tendency of an object to change its dimension either in length, density, area, or volume due to heat. When the substance is heated it increases its kinetic energy. Thermal expansion is of three types:

1. Linear expansion
2. Area expansion
3. Volume expansion

1.4 Literature Review

The 17 century witnessed enormous developments in experimental thermal science fostered by the invention of many new scientific instruments. One of these, Fahrenheit's mercury-in-glass thermometer, appeared at the beginning of the century and paved the way for much of the progress in thermal science. The work of skillful scientists and mechanicians provided the other tool necessary for the study of the thermal expansion of solids, namely devices to measure very small displacements. One person who particularly contributed to the development of experimental physics was W. J. Gravesande, a professor of astronomy at Leyden University. In his

book, Physices Elementa Mathematica Experimentis Confirmata, etc. (Mathematical Elements of Physics Confirmed by Experiments, etc., 1st ed. 1719-20) he described many experiments in the physical sciences. One, of particular historical interest, was the first experiment demonstrating the thermal expansion of solids. A brass ring, later called Gravesande's ring, allowed the passage of a brass sphere at room temperature while preventing passage after the sphere had been heated. An early inducement for the measurement of the Coefficient of Thermal Expansion resulted from precision time measurements [Ho and Taylor, 1998].

1.5 Present Work

Silicon is an ideal reference material for thermal expansion measurements, because it is isotropic in thermal expansion owing to its diamond-like crystallographic structure and because it is readily available in an ultra-pure condition as a result of the needs of the electronics industries [Watanabe et al., 2004]. Single crystal silicon is sometimes used as a standard, for instance for calibration of dilatometers as a material with a well-documented linear thermal expansion. Thus knowledge of the thermal expansion coefficient (CTE) of silicon versus temperature and crystallographic orientation is very important [Mazur and Gasik, 2009].

Copper is one of the most important materials in cryogenic engineering. It has many advantages as a structural material for cryogenic instruments, because of its very high thermal conductivity, high electric conductivity, machinability, weldability, etc. However, the linear thermal expansion coefficient (LTEC) is also a very important thermophysical property for cryogenic materials, as it is needed to estimate the thermal stress among

materials with different thermal expansion coefficients [Okaji et al., 1997]. The copper used in this investigation was Standard Reference Material 736 (SRM 736), supplied by The United States National Bureau of Standards. And has purity of 99.99%. This material is supplied with a Certificate of Analysis which gives values of expansion and expansivity in the temperature range 20-800 K. Third order polynomials are also given which describe the expansivity within three temperature bands [Bennett, 1978].

CHAPTER TWO

MATERIALS AND METHODS/THEORY

2.1 Thermal Expansion Theory

If energy is supplied to a solid, two phenomena take place: an increase in temperature and a change in volume; both of these are directly related to the increased vibrational energy of the molecules., thermal expansion caused by anharmonic terms in the restoring potential between the single molecules. The Debye model assumes that a solid is described by a set of harmonic oscillators. In this scenario, the oscillator frequencies in a perfect crystal (normal mode frequencies) are unaffected by change in volume, so no thermal expansion is predicted. From measurements, we know that this model is not correct. In fact, the introduction of anharmonic terms in the interaction potential is needed to get a positive volumetric coefficient of thermal expansivity [Ventura and Perfetti, 2014].

2.2 Definition

Thermal expansion is a consequence of the change in the average separation between the constituent atoms in an object. When the temperature of the solid increases, the atoms oscillate with greater amplitudes; as a result, the average separation between them increases. Consequently, the object expands. Considering a bar of length L_0 (Figure 1) to an initial temperature T_0, when the temperature ascends to a temperature T ($T > T_0$), the change of

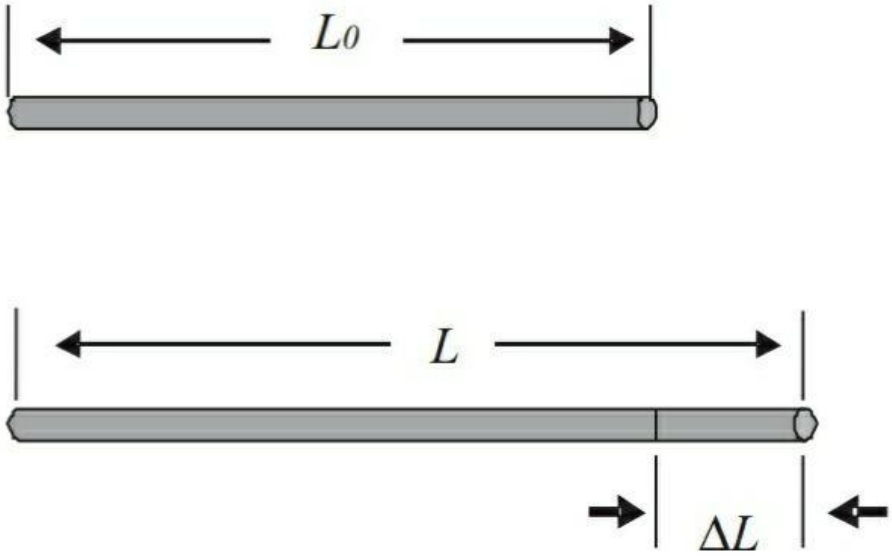
length $\Delta L = L - L_0$ is proportional to the change of temperature $\Delta T = T - T_0$ and the initial length L_0 ; this is:

$$\frac{\Delta L}{L_0} = \alpha_L \Delta T \qquad (1)$$

$$\alpha_L = \frac{\Delta L}{L_0 \times \Delta T} \qquad (2)$$

Where L_0 and L represent, respectively, the original and final lengths with the temperature change from ΔT. The parameter α CTE (Coefficient of Thermal Expansion) and has units of reciprocal temperature (K^{-1}) such as μm/m · K or 10^{-6}/K. The coefficient of thermal expansion is also often defined as the fractional increase in length per unit rise in temperature [Torres and Montero, 2009].

Figure 1 – Linear thermal expansion of a solid.



Area expansion occurs is the change in area due to temperature change. Area expansion formula is given as,

$$\frac{\Delta A}{A_0} = \alpha_A \Delta T \qquad (3)$$

$$\alpha_A = \frac{\Delta A}{A_0 \times \Delta T} \qquad (4)$$

Where A and A_0 represent, respectively, original and expanded area, ΔT is the temperature difference, ΔA is the change in the area, and α_A is the area expansion coefficient,

There is a corresponding change in volume, V_0 to V to describe this change the mean coefficient of volumetric thermal expansion of the material is defined by

$$\frac{\Delta V}{V_0} = \beta_{\mathrm{v}} \Delta T \qquad (5)$$

$$\beta_{\mathrm{v}} = \frac{\Delta V}{V_0 \times \Delta T} \qquad (6)$$

Where ΔV and V_0, are the volume change and original volume, respectively, and β, represents the volume coefficient of thermal expansion. In many materials, the value of β, is anisotropic; that is, it depends on the crystallographic direction along which it is measured. For materials in which the thermal expansion is isotropic, β, is approximately 3α [Touloukian et al., 1975].

2.3 Methods of Calculation

To determine the thermal expansion coefficient, two physical quantities (displacement and temperature) must be measured on a sample that is undergoing a thermal cycle. Three of the main techniques used for CTE measurement are dilatometry, interferometry, and thermomechanical analysis. Optical imaging can also be used at extreme temperatures. X-ray diffraction can be used to study changes in the lattice parameter but may not correspond to bulk thermal expansion.

Dilatometry. Mechanical dilatometry techniques are widely used. With this technique, a specimen is heated in a furnace and displacement of the ends of the specimen are transmitted to a sensor by means of push rods. The precision of the test is lower than that of interferometry, and the test is generally applicable to materials with CTE above 5×10^{-6}/K (2.8×10^{-6}/°F) over the temperature range of –180 to 900 °C (–290 to 1650 °F). Push rods may be of the vitreous silica type, the high-purity alumina type, or the isotropic graphite type. Alumina systems can extend the temperature range up to 1600 °C (2900 °F) and graphite systems up to 2500 °C (4500 °F).

Interferometry. With optical interference techniques, displacement of the specimen ends is measured in terms of the number of wavelengths of monochromatic light. Precision is significantly greater than with dilatometry, but because the technique relies on the optical reflectance of the specimen surface, interferometry is not used much above 700 °C (1290 °F). a standard method for linear thermal expansion of rigid solids with interferometry that is applicable from –150 to 700 °C (–240 to 1290 °F) and is more applicable to materials having low or negative CTE in the range of $<5 \times 10^{-6}$/K (2.8×10^{-6}/ °F) or where only limited lengths of thickness of other higher expansion coefficient materials are available.

Thermomechanical analysis. measurements are made with a thermomechanical analyzer consisting of a specimen holder and a probe that transmits changes in length to a transducer that translates movements of the probe into an electrical signal. The apparatus also consists of a furnace for uniform heating, a temperature-sensing element, calipers, and a means of recording results. the standard test method for linear thermal expansion of solid materials by thermomechanical analysis. The lower limit for CTE with

this method is 5×10^{-6}/K (2.8×10^{-6}/°F), but it may be used at lower or negative expansion levels with decreased accuracy and precision. The applicable temperature range is –120 to 600 °C (–185 to 1110 °F), but the temperature range may be extended depending on instrumentation and calibration materials [Cverna, 2002].

CHAPTER THREE

RESULTS AND DISCUSSION

3.1 Thermal Expansion of Silicon

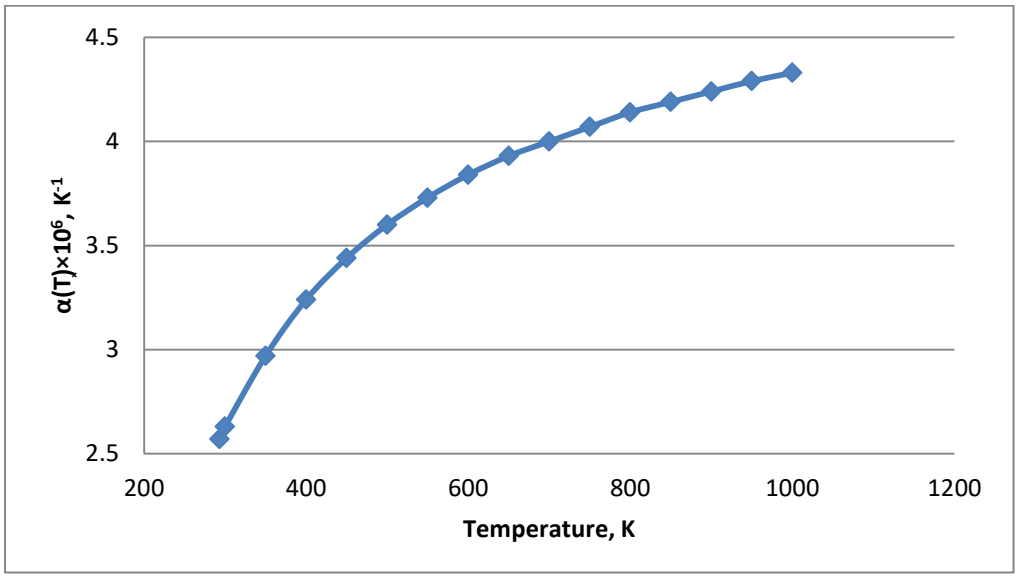
Table 1. Shows the experimental results for linear thermal expansion coefficient α(T) for single-crystal Silicon in temperature range 293 to 1000 K. Values of ΔL, ΔT, and L were measured with a heterodyne laser Michelson interferometer, a gold versus platinum (Au/Pt) thermocouple, and a linear gauge, respectively. Figure 2. Is plotted the linear thermal expansion coefficient α(T), of single-crystal Silicon as a function of temperature in degrees Kelvin. The curve is graphically obtained from the plot of data of Table 1.

Table 1 - Results of thermal expansion measurements for Silicon in temperature range 293 to 1000 K

Temperature T (K)	Linear thermal expansion coefficient $\alpha(T)\times10^{6}(K^{-1})$	Expanded uncertainty (k=2) $\delta\alpha(T)\times10^{6}$ (K^{-1})
293	2.57	0.038
300	2.63	0.039

350	2.97	0.040
400	3.24	0.042
450	3.44	0.043
500	3.60	0.045
550	3.73	0.045
600	3.84	0.046
650	3.93	0.047
700	4.00	0.044
750	4.07	0.045
800	4.14	0.045
850	4.19	0.046
900	4.24	0.046
950	4.29	0.048
1000	4.33	0.048

Figure 2 – Linear thermal expansion coefficient α(T) of Silicon as a function of temperature.



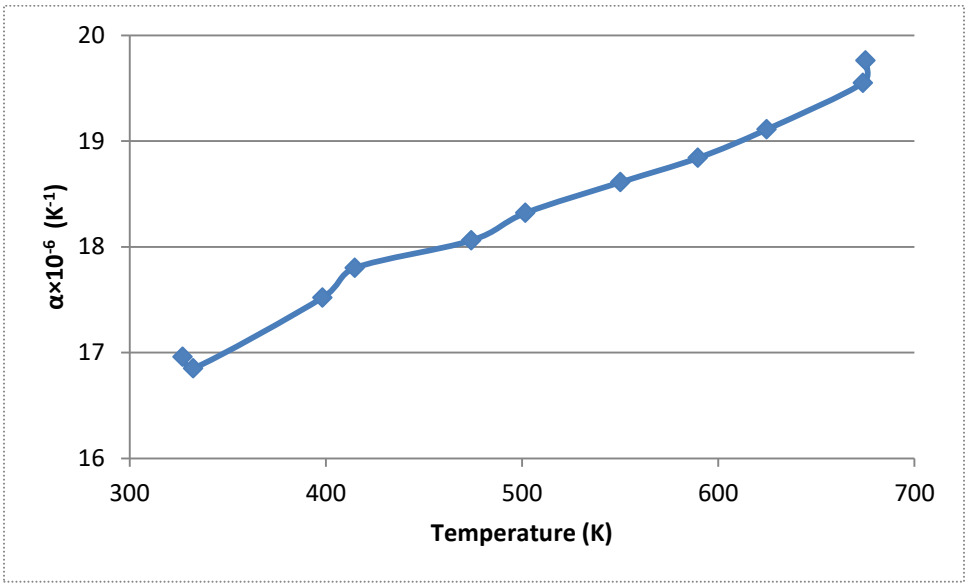
3.2 Thermal Expansion of Copper

Table 2. Shows the experimental results for linear thermal expansion coefficient α(T) for Copper Standard Reference Material 736 (SRM 736) The expansion was measured in an interferometric dilatometer within the range 300 to 700 K. Linear thermal expansion coefficient σ(T) of Copper were obtained from Table 2. Are plotted in Figure 3. As a function of temperature in Kelvin.

Table 2 - Results of thermal expansion measurement for Copper in temperature range 300 to 700 K

Temperature T (K)	Linear thermal expansion coefficient $\alpha(T) \times 10^{-6}$ (K^{-1})
327.1	16.96
332.5	16.85
398.4	17.52
414.8	17.80
474.2	18.06
501.8	18.32
550.2	18.61
589.7	18.84
624.8	19.11
673.8	19.55
675.2	19.76

Figure 3 – Linear thermal expansion coefficient α(T) of Copper as a function of temperature.



CHAPTER FOUR

CONCLUSION AND FUTURE WORK

4.1 Conclusion

Linear thermal expansion data, α(T), on single-crystal silicon in the temperature range 293 to 1000 K have been determined using a laser interferometric dilatometer. The expanded uncertainties (k=2) of α(T) in the measured temperature range were estimated to be 3.8×10^{-8} to 4.8×10^{-8} K^{-1}. The respective standard deviations of the measured α(T) were estimated to be 7.5×10^{-9} K^{-1}, which were within the magnitudes of their expanded uncertainties. The present results are in good agreement with the most recently reported data [Watanabe et al., 2002:pp.548-549] but not with the earlier reported data at temperatures above 700 K [Okaji, 1988:pp.1104-1105], both of which were measured with the dilatometers similar to that used in the present work. The poor agreement with the earlier reported data, which were used to estimate the present CODATA recommended values [Ho and Taylor, 1998:pp.277], suggests the need for a reevaluation of the standard reference values of α(T) on silicon at temperatures above 600 K.

Measurements of the thermal expansion of the NBS copper reference material SRM 736 have indicated good agreement with the NBS calibration between 300 and 600 K. Above 600 K, values have been obtained which indicate that the NBS calibration may be low, The three calibrations agree within 0.5% between 300 and 630 K and within 2.5% above 630 K. In order to resolve these remaining differences, further measurements should be

undertaken to establish a generally accepted calibration for the whole temperature range, and particularly above 600 K.

4.2 Future Work

1. The investigation of thermal expansion in Germanium
2. Band Structure of Silicon for bulk and nano
3. Effect of size on band gap energy in nano particles

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