JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 15, No. 1, January–March 2001

Prediction of Thermal Contact Conductance in Vacuum Using Monte Carlo Simulation

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Predictions of thermal contact conductance between two conforming flat surfaces in vacuum are carried out. The prediction model considers heat flow through the contact zones of asperities on the surfaces by conduction. The probability of occurrence of contact between the surface asperities is evaluated using a Monte Carlo simulation. A Gaussian distribution of asperity heights on the surfaces, which has been validated earlier, is assumed. The distribution of these contact spots and their respective contact areas are determined in the model and used for evaluating the thermal contact conductance. Predictions are carried out for different materials at varying contact pressures in a vacuum environment. A wide range of surface characteristics is considered. The predictions show excellent agreement with the measured values of thermal contact conductance.

Nomenclature

A	=	area, m^2
a	=	radius of contact spot, m
b	=	radius of an adiabatic channel for a given contact point, m
H	=	microhardness of the softer material, Pa
h	=	thermal contact conductance, W/m^2 K
h^*	=	nondimensional contact conductance
k	=	thermal conductivity, W/mK
m	=	slope of the asperity
N	=	total number of asperities
N_T	=	density of asperities, per m^2
n	=	number of uniform random number
P	=	contact pressure, Pa
P^*	=	nondimensional contact pressure
Q	=	heat flow rate, W
S	=	sum of n uniform random numbers
U_x	=	Gaussian random number
x	=	summit height, m
ΔT	=	temperature difference
δ	=	summit penetration depth, m
ε	=	clearance between the surfaces, m
μ	=	mean roughness, m
σ	=	standard deviation in summit heights, m
ψ	=	constriction alleviation factor

Subscripts

a	=	apparent
c	=	contact
G	=	Gaussian distribution
i	=	ith asperity
max	=	maximum
r	=	real
1, 2	=	surfaces 1 and 2

Introduction

ALL solid surfaces are characterized by certain degree of roughness. Two solid surfaces in contact will touch each other only at a few points, depending on the degree of the surface roughness. Even at relatively high contact pressures, the actual area of contact for most metallic surfaces is less than about 2% of the nominal contact area.[1,2] The small contact area impedes the flow of heat across the interface and introduces thermal resistance at the joint. This resistance, known as thermal contact resistance, manifests itself as a sudden temperature drop at the interface. This is schematically shown by ΔT_c in Fig. 1. When the interstitial material at the joint is a poor heat conductor, such as air, the heat flow lines converge to the discrete solid–solid contact spots as illustrated in Fig. 2. Convection and radiation heat transfer at the joint is negligible.[3] However, the heat flow through the gaps cannot be neglected if the solids are relatively poor conductors.

The thermal contact conductance, also known as solid spot conductance and denoted by h, is defined as the ratio of the heat flux Q/A to the additional temperature drop ΔT_c, shown in Fig. 1, due to the presence of the joint. It is given by

$$h = Q/(\Delta T_c A) \tag{1}$$

There are several applications where a low value of thermal contact conductance is desirable. These include low-conductivity structural supports for storage and transport of cryogenic fluids and thermal isolation joints for spacecraft components. It is necessary to be able to design joints for specified values of thermal contact conductance. This is specifically required for small-scale heat removal systems such as in microelectronics[4,5] and heat transfer between superconductor films and substrates.[6] Other areas of application include thermal rectification[7] and conductance enhancement by metallic coatings.[8,9]

A number of theoretical and experimental studies of the thermal contact conductance between two conforming metallic surfaces have been reported in the literature.[2–7] The theoretical studies are based on the consideration of heat flowing through one microscopic contact region and extending it for the surface using a constriction alleviation factor.[2] In the absence of heat transfer via the interstitial medium and heat transfer by radiation, the heat flow across a pressed contact occurs across the distributed microcontacts. Yovanovich[10] assumes that the contacting asperities undergo plastic deformation. The Vicker's microhardness is used to relate the actual contact area and the applied pressure. The methodology reasonably predicts the values of contact conductance of pressed joints.

The number and average size of the numerous microcontacts need to be known to a priori predict the thermal contact conductance. Greenwood and Williamson[11] proposed one of the first contact models to incorporate the statistical nature of the contact between two surfaces.

More recently, Leung et al.[12] developed a statistical model for predicting the contact conductance for nominally flat surfaces. The physical foundation of this statistical approach is based on the analogy that surface asperities are comparable to particles in the

Received 22 March 2000; revision received 20 July 2000; accepted for publication 21 July 2000.

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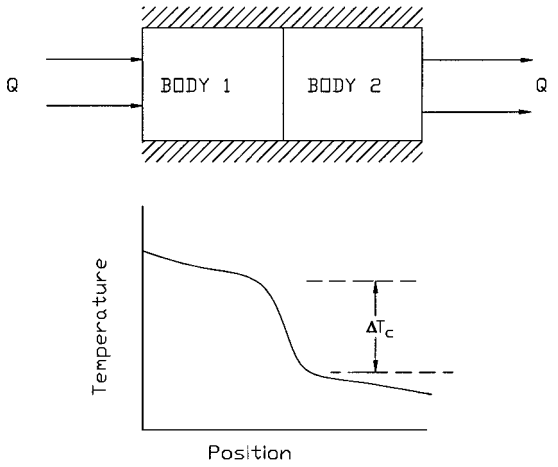

Fig. 1 Schematic of heat conduction at interface.

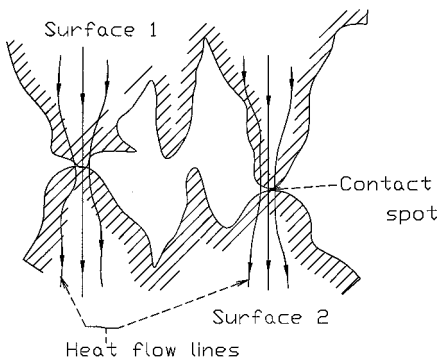

Fig. 2 Profiles of contacting surfaces and heat flow across contacts.

traditional sense of a microscopic viewpoint. The Boltzman statistical model is applied to determine the most probable distribution of asperity heights for a homogeneous, isotropic rough surface. The analysis showed the distribution of contact points to be Gaussian, which was assumed earlier but not rigorously substantiated. A relationship was derived, using Boltzman statistical analysis, for the thermal contact conductance as a function of pressure at the joint. This correlation could predict contact conductance within about 30% of the experimental data.

The influence of roughness and waviness has been studied by Yovanovich.[13] Predictions of thermal contact conductance for nominally flat surfaces were carried out by Hsieh.[14] Hsieh also developed correlations for thermal contact conductance and made a critical evaluation of the role of surface geometrical parameters for a nominally flat surface model. Yovanovich[10] developed theoretical relationships for determining contact, gap, and joint conductances for conforming rough surfaces and found reasonably good agreement between theoretically predicted and measured values.

The existing predictions are based on phenomenological models using experimental inputs. The contact resistance is due to the reduced area of contact of the surfaces. The contact surface area can be determined from the number of contact points and their respective areas, following which the thermal contact conductance can be predicted. This approach is adopted in the present investigation.

A simple but potentially promising simulation procedure of Monte Carlo using random numbers is applied to estimate theoretically the thermal contact conductance. Junctions formed by two flat dissimilar or similar materials in a vacuum are considered. The distribution characteristics of the asperities are combined with a Gaussian random number approach to define the probability of the height of the asperities and the nature of the contact between the asperities of the two surfaces in contact with each other. The thermal contact conductance is determined for a given interfacial pressure from the number and surface area of the contact spots, when consideration of the plastic deformation of asperities is taken into account. The approach is promising in view of the simplicity in the formulation of the macroscopic contact probabilities and the versatility of accommodating different contact surface geometries.

Theoretical Formulation

All three modes of heat transfer, namely, conduction, convection, and radiation, prevail across a pressed contact. Energy transfer primarily occurs by radiation and conduction through the interstitial medium and by conduction through the microcontacts. At relatively low temperatures ($\leq$500 K), the heat transfer across pressed contacts, located within a vacuum environment ($<10^{-3}$ torr), would be dominated by conduction through the actual contact area.[15] In the following, the problem of contact conductance for joints in vacuum at low temperature is formulated. The following geometrical, physical, and thermal assumptions are made:

1) The surfaces are microscopically rough and macroscopically conforming.

2) The distribution of asperity heights is Gaussian and the asperities are randomly distributed over the apparent contact area.

3) The contacting asperities deform plastically during loading, and the deformation occurs in the softer solid.

4) As a result of the deformation, there are N circular contact spots within the apparent area A_a having a contact radii a_i. An equivalent circular flow tube of radii b_i is associated with each contact spot[16] and is shown in Fig. 3.

5) Radiative heat transfer is negligible and the surfaces are free of oxides or other films.

The heat flow under steady-state conditions across the joint will be distributed among the contact spots of different sizes existing at the contact plane. With the assumption that the contact point is circular with a radius a_i, the heat flow rate for each individual contact can be written as[17]

$$Q_i = 2ka_i \Delta T_c (1/\psi_i) \tag{2}$$

where ΔT_c is the temperature drop across the interface. For geometrically similar contacts (i.e., when the contact plane is the surface of symmetry), ΔT_c is the same for all contact points. Here, ψ_i is a geometrical factor equal to unity for a single contact belonging to an infinite apparent area. The value of the geometrical factor has been exmained by different authors, both analytically and numerically.[18–20] For appropriately distributed contacts having contact points at the center of mating asperities, a simple expression that closely approximates the analytical and numerical solution is given by[21]

$$\psi_i = [1 - (a_i/b_i)]^{1.5} \tag{3}$$

In the preceding equation, a_i/b_i can be replaced[21] by $(P/H)^{0.5}$. When the variation in ψ is neglected from contact to contact, the value of ψ becomes

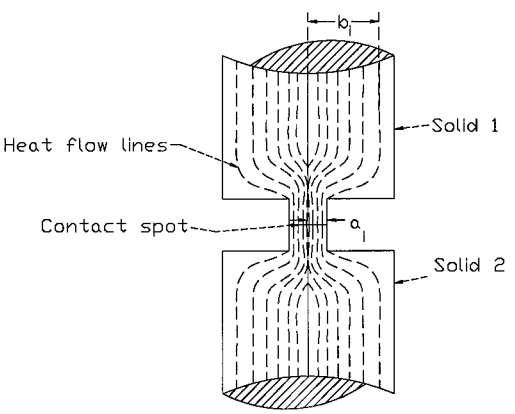

Fig. 3 Construction of heat flow tube at contact spot.

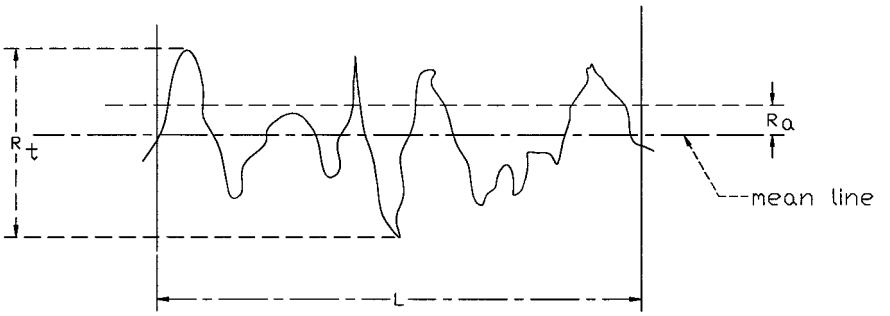

Fig. 4 Definition of roughness parameters R_a and R_t.

$$\psi = \left[1 - \sqrt{P/H}\right]^{1.5} \tag{4}$$

Heat flow per unit apparent area A_a is given by

$$\frac{Q}{A_a} = \sum \frac{Q_i}{A_i} = 2k\Delta T_c \sum \frac{a_i/A_a}{\psi_i} \cong \frac{2k\Delta T_c}{\psi A_a} \sum a_i \tag{5}$$

The thermal contact conductance h can be determined from the preceding equation to be

$$h = \frac{Q/A_a}{\Delta T_c} = \frac{2k}{\psi A_a} \sum a_i \tag{6}$$

The value of

$$\sum a_i$$

is obtained from consideration of the surface parameters and is detailed in the following sections.

Surface Representation

The surface roughness is usually characterized by an average surface roughness value R_a and a peak-to-valley surface roughness value R_t. Figure 4 illustrates these two characteristic roughness parameters. Whereas R_a gives the arithmetic average heights of the protrusions about the mean reference plane, R_t gives the maximum peak-to-valley roughness height measured parallel to the mean line.

The distribution of the asperity heights is assumed to be Gaussian. This is based on the extensive experimental observation of actual surfaces.[11,22,23] Predictions[12] made using a Boltzman statistical model showed that the most probable distribution of asperity heights for a homogeneous, isotropically rough surface is Gaussian in nature. The distribution is given as

$$f(x) = \left(1/\sqrt{2\pi}\sigma\right) \exp\left\{-\tfrac{1}{2}[(x-\mu)/\sigma]^2\right\} \tag{7}$$

In the present study, the surface parameters are described by a standard deviation for combined height distribution σ and an average absolute slope $m = \tan\theta$.

The irregularities on the rough surface are modeled as conical asperities of identical gradients m and various heights, resting on a common flat plane, and are illustrated in Fig. 5. This model[14] has been shown to be a good representation of surfaces prepared by grinding, lapping, honing, bead blasting, anodizing, and accurate casting. The summit height distribution given by Eq. (7) leads to some useful characteristics[14] of the number of asperities and their heights as given in the following. The density of surface asperities (number per unit area) is

$$N_T = (m/7.308\sigma)^2 \tag{8}$$

Maximum summit height (peak-to-valley roughness R_t) is

$$x_{\max} = 8\sigma \tag{9}$$

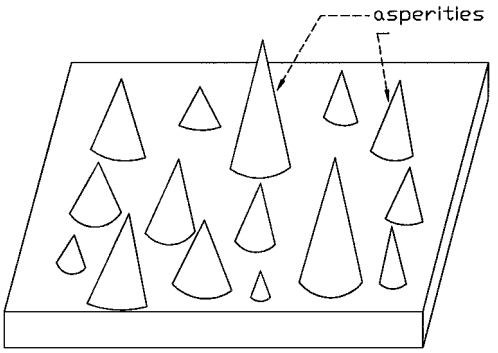

Fig. 5 Rough surface model with conical asperities.

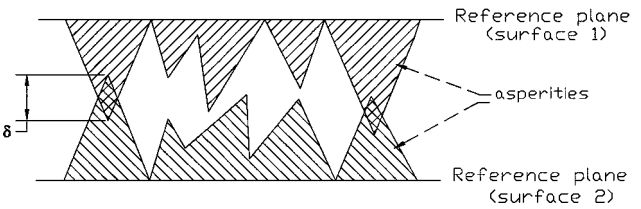

Fig. 6 Rough surface contact model.

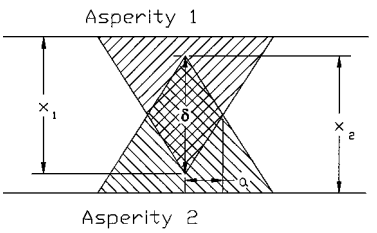

Fig. 7 Idealized contact element.

The mean summit height is

$$\mu = 4\sigma \tag{10}$$

Note that the asperities having heights beyond $x_{\max}$ are less than 0.02% (negligibly small) of the total population described by Eq. (7) (Ref. 12).

The formation of the true contact areas is modeled following the scheme shown in Fig. 6. The first step in modeling is to represent each rough surface by the conical asperities. Perfect alignment between a pair of touching asperities rarely occurs. Nevertheless, the degree of misalignment is expected to be statistically constant because the macroscopic properties such as the thermal contact conductance and the surface friction are reproducible.[12] It has also been reported that the theoretical prediction of thermal contact conductance can be corrected, if necessary, by a multiplying factor, which is close to unity as shown by Hsieh.[14]

The fundamental unit for the study of conductance at an interface is a single contact formed by a pair of touching asperities shown in Fig. 7. In the mechanical analysis, touching asperities "resemble blunt indentures whose summit undergoes a plastic deformation."[12]

Based on simple geometry, this mechanism results in the contact spot radius

$$a = 0 \quad \text{if} \quad \delta \le 0$$
$$= \delta/2m \quad \text{if} \quad \delta > 0 \tag{11}$$

where δ is the summit penetration depth depicted in Fig. 6. A value of δ less than zero implies that the two asperities are not in contact.

When both sides of the contact spot are made of dissimilar materials, the total resistance is simply the sum of the resistances for each side of the contact. Therefore, if k_1 and k_2 are the thermal conductivities of the two solids in contact, then the equivalent conductivity k (to be used in the equation to estimate h) is taken as the harmonic mean of the conductivities:

$$k = 2k_1k_2/(k_1 + k_2) \tag{12}$$

Similarly, if the conforming surfaces have different standard deviations of asperity heights σ_1 and σ_2 and respective slopes of $\tan\theta_1$ and $\tan\theta_2$, then their equivalent values are taken as

$$\sigma = \left(\sigma_1^2 + \sigma_2^2\right)^{0.5} \tag{13}$$

$$\tan\theta = \left(\tan\theta_1^2 + \tan\theta_2^2\right)^{0.5} \tag{14}$$

The separation distance between the reference planes of the two conforming surfaces, otherwise denoted as the average clearance between the surfaces, is given by

$$\varepsilon = \sqrt{2}\sigma\,\text{erfc}^{-1}(2A_r/A_a)$$
$$= \sqrt{2}\sigma\,\text{erfc}^{-1}[2P/(P + H)] \tag{15}$$

In the preceding expression, A_r/A_a is approximated for plastic deformation as $P/(P + H)$ following Mikic.[17] This assumption has been shown[2,17] not to introduce significant errors for the contact pressures that are of general interest in practical applications.

Monte Carlo Random Number Approach

The probabilistic nature of the surface characteristics is simulated using random numbers. The respective surface asperity heights, nature of contact, and their distribution are considered. The main objective is to find out the number of contacts and their respective contact spot radii a_i.

Number of Contacting Asperities

For two contacting surfaces having same surface texture, the number of asperities in an area A_a is given by

$$N = N_T \times A_a \tag{16}$$

The height of an asperity randomly located on either surface could vary between 0 and $x_{\max}$. The individual heights would follow a Gaussian distribution. If $x_{\max 1}$ and $x_{\max 2}$ are the respective maximum asperity heights of the mating surfaces 1 and 2, and if we choose randomly one asperity each on either surface of height x_1 and x_2, then

$$x_1/x_{\max 1} \le 1 \tag{17}$$

$$x_2/x_{\max 2} \le 1 \tag{18}$$

The ratio of $x_1/x_{\max 1}$ and $x_2/x_{\max 2}$ could take any Gaussian random number U_x between 0 and 1, that is,

$$x_1/x_{\max 1} = U_{x1} \tag{19}$$

$$x_2/x_{\max 2} = U_{x2} \tag{20}$$

Now, by randomly assigning two Gaussian random numbers for U_{x1} and U_{x2} for the two preceding expressions, the individual asperity heights of the conforming surfaces can be estimated. An idealization that is made here and that was discussed earlier is that these two asperities are facing each other with perfect alignment. The errors associated with the assumptions are discussed subsequently.

The clearance between the surfaces, which depends on the surface characteristics and on the applied pressure and material hardness, is given by Eq. (15). This is applicable only for $A_r/A_a < 0.5$. Clearance would be negligible if A_r/A_a is greater than 0.5. Studies have shown[1,2] that in almost all applications this ratio is well below 0.5.

If the combined heights of the asperities is larger than the clearance, then these asperities will touch each other. Accordingly, if

$$x_1 + x_2 > \varepsilon \tag{21}$$

a contact is made between the asperities. A contact counter is opened that increments for the each additional contact that is made, namely, $n_c = n_c + 1$.

Interface Area of Contacting Asperities

Having estimated the number of contacting asperities between the surfaces, the area of their respective contact zones is to be determined.

The penetration depth of the asperity is given by

$$\delta = x_1 + x_2 - \varepsilon \tag{22}$$

where ε is the clearance between the surfaces.

Once δ is known, the spot contact radii a_i (Fig. 7) can be calculated from the expression [Eq. (11)] derived earlier. The method is repeated for all of the asperities in the region N. At the end of this exercise, the total number of contact spots and their respective contact radii are known.

In the preceding analysis, Gaussian random numbers are generated from a set of uniform random numbers. The Gaussian random number generator uses the following expression for the analysis:

$$U_x = (S - n/2) \times \sigma_G \times \sqrt{12/n} + \mu_G \tag{23}$$

Here, σ_G and μ_G are derived, respectively, from the standard deviation σ and mean μ of the surface roughness characteristics. This is done by transforming the Gaussian distribution of asperity heights to a Gaussian random number distribution between 0 and 1 and equating the peak value to $8\sigma_G$, where σ_G corresponds to the standard deviation of the required random number distribution.

Results and Discussion

The Microsoft FORTRAN uniform random number generator subroutine RANDOM is used for generating Gaussian random numbers for defining various probability functions. This subroutine returns a variable whose value varies between 0 and 1 for an input seed value. The computer program was written in FORTRAN-77 and run on a Pentium class 350-MHz machine. A typical run with a surface having roughness R_a of 0.125 μm took about 820 CPU s. The accuracy of the predictions was verified by repeating the computation for the same input seed value used for the generation of uniform random numbers. The results reproduced within 0.1%. When the number of random numbers used for the generation of Gaussian random numbers was doubled, the deviations were found to be even smaller. The relative difference in the estimated values of conductance for double precision and single precision calculations was less than 0.16%. The dispersions showed a marginal increase when very rough surfaces were considered.

To assess the robustness of the model and the suitability and accuracy of the predictions, the estimated values of contact conductances are compared with the existing experimental data[16,24] in Fig. 8. The experimental data are for two different stainless steel materials (SS416 and SS303) under vacuum obtained at different values of applied pressure. The contact conductance varies almost linearly with the applied pressure. Also note that variations in the predicted values and measured data are within the uncertainty in the experimental data. However, the plot may not be a direct representation of the material properties alone because the materials under test had different surface characteristics.

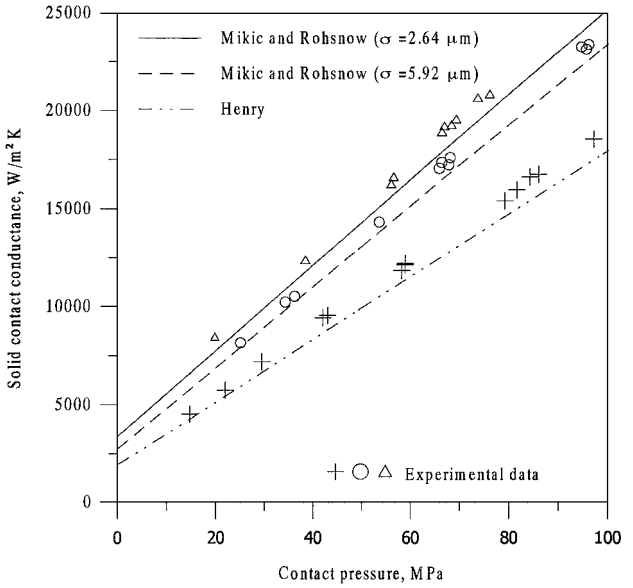

Fig. 8 Comparison of predictions with experimental data.

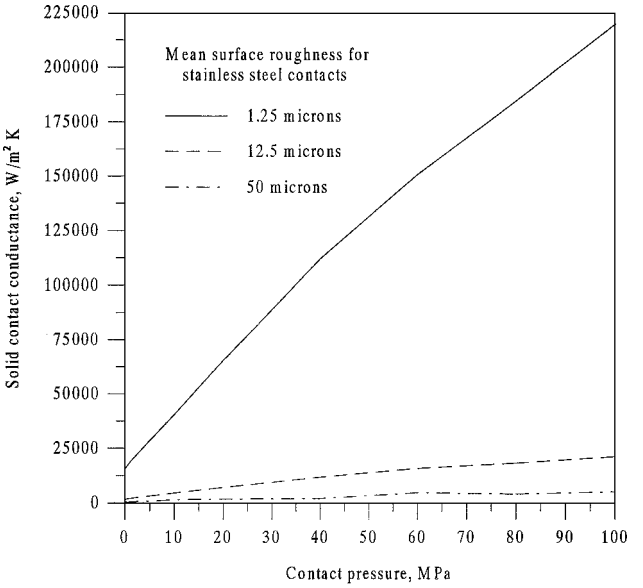

Fig. 10 Influence of surface roughness on thermal contact conductance.

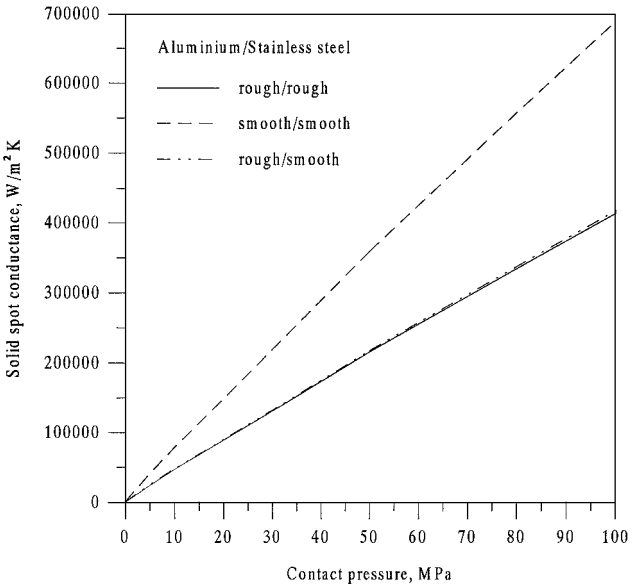

Fig. 9 Variation of contact conductance with changes in contact pressure and surface roughness.

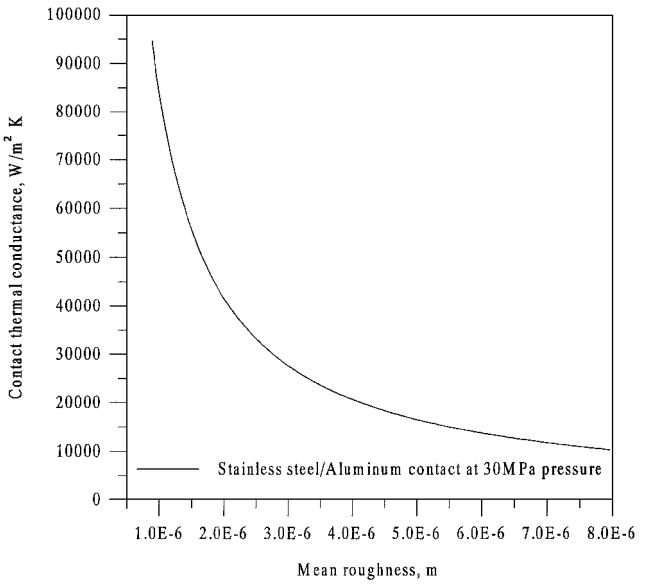

Fig. 11 Nondimensional representation of thermal contact conductance.

The analysis was further extended for three different cases of surface roughness with the material combination of aluminum and stainless steel. Three values of roughness parameters of the two surface were chosen, namely, 1) 1.25 μm and 1.25 μm (rough/rough), 2) 0.125 μm and 0.125 μm (smooth/smooth), and 3) 1.25 μm and 0.125 μm (rough/smooth). The estimated values of thermal contact conductance for these combinations for various applied loads are illustrated in Fig. 9. As expected, the smooth/smooth combination gave highest values of conductance, whereas a rough-to-rough surface and rough-to-smooth surface combination gave lower values that were almost similar. For smooth surfaces, the number of asperities in contact is high, and, therefore, the actual area of contact is higher and thereby results in higher contact conductance values. On the other hand, when the rough surfaces are in contact, there is a higher number of asperities that are not in contact. This results in a lower value of thermal contact conductance. The conductance values coincide with those of a rough surface joined to a smooth surface. This is because in the present study only plastic deformation of the asperity is considered and its flow is not considered. Under pressure, the softer metal deforms against the harder metal leading to identical values of thermal contact conductance for the rough/rough and rough/smooth surface. This observation is in agreement with the findings of other researchers.[2]

Figure 10 shows the predicted values of surface contact conductance for stainless steel contacts having same roughness parameters on either side. Results again show that smooth surfaces give higher values of conductance compared to rougher surfaces. For very rough surfaces with surface roughness parameter $R_a = 50$ μm, the thermal contact conductance values do not vary significantly with changes in applied pressure.

The significance of the changes in thermal contact conductance due to the changes in the surface roughness is further highlighted in Fig. 11. Calculations were carried out for a stainless steel/aluminum contact under 30 MPa contact pressure with different mean surface roughness values. A rapid reduction in contact conductance is seen when the surface roughness changes from smooth to moderately rough. The changes are less pronounced, and the conductance values tend to insignificant levels for very rough surfaces. Note that surfaces having very high mean roughness will have lot of void spaces even at high contact pressures, resulting in the low values of conductance.

In all, some 79 sets of data on thermal contact conductance were obtained by varying surface parameters, material properties, and contact pressure. They are nondimensionalized for the thermal contact conductance and contact pressures. The dimensionless contact conductance is given by

$$h^* = (h\sigma/m)/k \tag{24}$$

Because the length scale σ/m is representative of the total contact area made between the asperities, the term $h\sigma/m$ in the preceding expression is proportional to the equivalent thermal conductivity arising from the reduced contact area at the interface of the contacting surfaces. Therefore, the dimensionless thermal contact conductance is a measure of the reduced heat transfer due to the interface.

The dimensionless pressure is defined by

$$P^* = P/H \tag{25}$$

The dimensionless pressure term takes into account the material hardness. The preceding dimensionless parameters have been used in previous correlation studies.[12,21,25]

A least-squares fit of the predictions gives the following correlation:

$$h^* = 0.128 \times (P^*)^{0.651} \tag{26}$$

The load exponent of 0.651 is valid over the range of dimensionless loading parameter P^* between 0.002 and 0.1. The standard error in the h^* estimate is 0.008.

The load exponent of 0.651 is much lower than the theoretically derived value of 0.95 by Yovanvich.[10] A summary of load exponents used in the earlier correlations for thermal contact conductance for nominally flat surfaces in vacuum is reported by Leung et al.[12] These are given in Table 1 (see Refs. 10, 12, and 25–32).

Note that the exponent of 0.651, arrived at in the present set of predictions, is in close agreement with the experimental investigations of Edmonds et al.,[26] Ma'lkov,[27] Madhusudana and Fletcher,[28] and those reported by Leung et al.[12] using statistical mechanics.

Experimental data for stainless steel,[16,24] nickel 200 (Ref. 29), zirconium[29] and zircoloy[29] with the surface roughness variations between 0.338 μm (smooth) and 9.86 μm (rough) are shown in Fig. 12 along with the predictions of the present study in dimensionless form. Note that the predictions compare very well with the experimental results[16,24] over a wide range of pressures.

The maximum deviation of the prediction from the experimental data seems to be about 14% when the data of Hegazy[29] over a range of P^* are considered. However, they are found to match well with the prediction when P^* are less than 0.006. For higher values of P^*, the model tends to underpredict the contact conductance and the deviations increases with P^*. Note that the experimental data of Hegazy[29] at higher dimensionless contact pressures also do not agree well those reported[12,16,24] earlier.

Overall, the model underpredicts thermal contact conductance, especially at large values of contact pressures. The reason for the underprediction could be traced to the assumption that all contacting asperities are in perfect centerline alignment. In reality, there will be asperities having sliding contact with one another without undergoing any deformation, thus creating a higher area of contact than those available by centerline contact alone. This would explain the lower estimates of the thermal contact conductance.

Table 1 Load exponent values reported in literature

Reference	Load exponent
Yovanovich[10]	0.95
Hegazy[29]	0.95
Edmonds et al.[26]	0.60
Popov[30]	0.956
Thomas and Probert[31]	0.743–0.72
Fletcher and Gyorog[32]	0.56
Mal'kov[27]	0.66
Tien[25]	0.85
Leung et al.[12]	0.693
Madhusudana and Fletcher[28]	0.66

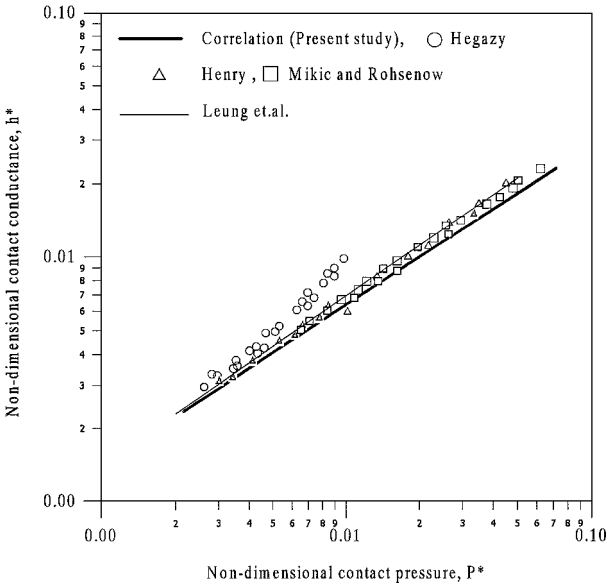

Fig. 12 Comparison of predictions with experimental data in dimensionless form.

Conclusions

Excellent prediction of thermal contact conductance using the Monte Carlo simulation procedure is demonstrated. The most probable distribution of contact spots is determined in the model, following which a relationship between the thermal contact conductance and the pressure is derived. Explicit dependence of contact conductance on surface roughness and the materials of contact is determined.

The predictions agree well with the measured data on thermal contact conductance published for different materials of varying surface roughness under different contact pressures. The theory constitutes a viable tool for the heat transfer analyst. It is relatively easy to implement, and the results are demonstrated to be accurate. A least-squares fit of the predicted data gives a correlation with the exponent of the load factor being 0.651. The work brings to focus the potential application of Monte Carlo approach for accurate prediction of thermal contact conductance.

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